Instrumentation

Infrastructure Improvements

DANCE—A Detector for Advanced Neutron Capture Experiments

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A new instrument for nuclear-physics research is being built on flight path (FP) 14 at the Lujan Neutron Scattering Center (Lujan Center). This state-of-the-art instrument, called DANCE (i.e., Detector for Advanced Neutron Capture Experiments), consists of a shell of 160 BaF_2 crystals, each 15 cm long, with an inner radius of 17 cm. DANCE will be used to study the neutron-induced transmutation of radioactive elements. This process is of interest in understanding the synthesis of the elements in stars, in studying the burn-up of nuclear waste, and in gaining a better understanding of archived data from past tests of nuclear explosives. Los Alamos National Laboratory (LANL) is unique in the world in being able to make these measurements.

Why Study Neutron Capture Today?

Neutron capture is a reaction in which a neutron strikes and sticks to a target nucleus, forming a new isotope. An example of this type of transmutation reaction is the absorption of a neutron by the element ^{171}Tm to form ^{172}Tm. Usually, this new isotope is not in its ground state (the lowest energy state of a nucleus), but it rapidly decays to its ground state by emitting a cascade of gamma (γ) rays, which are observed by a γ-ray detector such as DANCE.

The probability, or cross section, for neutron capture varies with the neutron energy. This probability has been measured on most stable nuclei over a wide range of neutron energies. However, theoretical calculations of the reaction probabilities can only predict these measurements to within a factor of 2. Because calculations do not provide sufficient accuracy, measurements of neutron capture on these radioactive nuclei are needed, and exceedingly few measurements have been made.

The neutron energies of interest are typically from 1 keV to near 1,000 keV. The water moderators at the Lujan Center provide an excellent source of neutrons in this energy range.

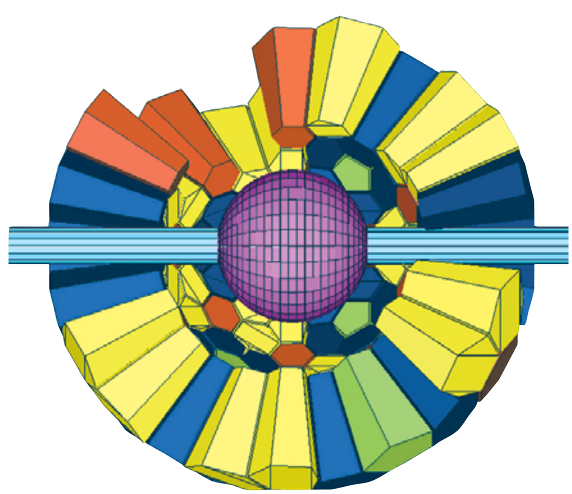
DANCE Will Use Unique Capabilities at LANL

The advanced detector that we are building is only one of the facilities required for these important neutron-capture experiments. The intense, pulsed neutron source of the Lujan Center is required to make measurements on small quantities of target material. Preliminary measurements using less efficient detectors have been made on 1-mg samples of the unstable nuclei ^{171}Tm and ^{150}Sm. The radioactive material handling and fabrication facilities of the Chemistry (C) Division at LANL, including the new Radioactive Species Isotope Separator, will be used to safely fabricate targets. The location of the three components necessary to make capture measurements on radioactive targets—target fabrication facilities, an intense neutron source, and an advanced detector—at LANL is unique in the world.

Measuring Neutron Capture

DANCE was designed to have high efficiency for γ-ray detection, to have good neutron-energy resolution, and to be relatively insensitive to experimental backgrounds. Extensive Monte Carlo calculations were done to aid in the design process.[1-3]

To meet these requirements, we are building a 162-segment, BaF_2 crystal array. Four different crystal shapes are required to completely cover the surface of a sphere with 162 equal-area segments, much like two different shapes are required in a 32-panel soccer ball. Two segments are left blank for the beam to enter and exit the array. This geometry is shown schematically in Fig. 1. The complete BaF_2 crystal array will have an

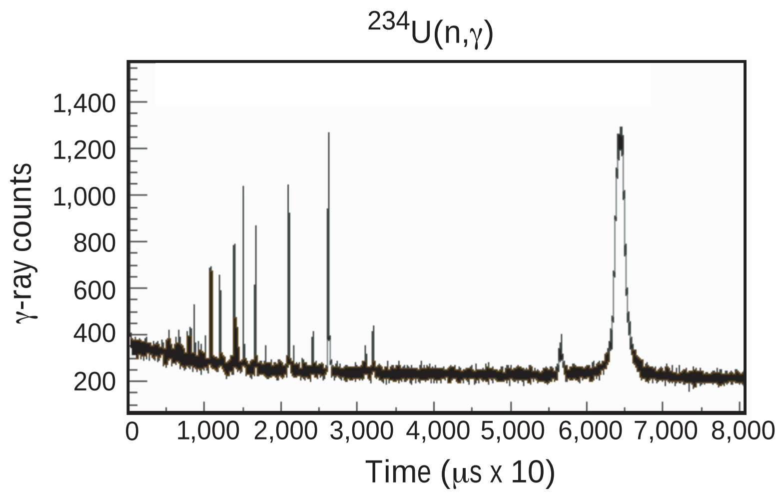


↑ ***Fig. 1.*** *A schematic of DANCE. Each color represents a different crystal shape. Four different shapes are required.*

inner radius of 17 cm, and each crystal is 15 cm long. There is space for a 6-cm-thick neutron absorber between the inner surface of the BaF_2 crystal array and the beam pipe.

The targets to be studied are located 20.26 m from the neutron moderator. The beam spot at that location has a radius of 0.3 cm. The BaF_2 crystal array can be opened in two sections to install the radioactive targets, which will be prepared at C Division's radioactive-isotope-handling facilities and transported to the Lujan Center.

The mechanical support for the advanced detector has been constructed, and the 160 BaF_2 crystals are arriving from the manufacturer. A new data-acquisition system using fast transient digitizers has been procured. We anticipate completion of the full array in the fall of 2002. First beam was taken down FP14 in September 2001. Several preliminary targets were studied in 2001, using existing C_6D_6 γ-ray detectors. Fig. 2 shows some preliminary first-ever capture data on ^{234}U taken over this energy range (i.e., 1 to 1,000 keV).



↑ ***Fig. 2.*** *Preliminary time-of-flight spectrum of neutron-capture data on ^{234}U from 0 to 800 μs taken at FP14 using C_6D_6 detectors. This represents the first measurement of this reaction over this energy range (i.e., 1 to 1,000 keV).*

References

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FIGARO—A Fast Neutron-Induced Gamma-Ray Observer

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Understanding nuclear reactions is key to reliable calculations of nuclear weapons, transmutation of radioactive waste from power reactors, and synthesis of the elements in stars. These calculations depend on accurate input parameters (generally more than twenty), some of which are fairly well known, but others are uncertain by uncomfortably large factors. Progress in narrowing down the range of possible parameters depends on new types of experimental data chosen judiciously to provide the necessary understanding of the reactions. We have constructed the new Fast Neutron-Induced Gamma-Ray Observer (FIGARO) instrument on a flight path at the Weapons Neutron Research Facility (WNR) to measure γ-ray and neutron-emission spectra following neutron-induced reactions to provide a new type of data to constrain the calculations. In addition, neutron emission from fission can be studied to provide data directly for applications.

Using FIGARO to Study Neutron-Induced Reactions

FIGARO is a flexible facility at WNR for the study of neutron-induced reactions that result in the emission of γ-rays and neutrons. We enhanced its capabilities in 2001 by adding more neutron detectors, and we made measurements heretofore not possible over a continuous wide range of neutron energies from 1 MeV to more than 100 MeV.

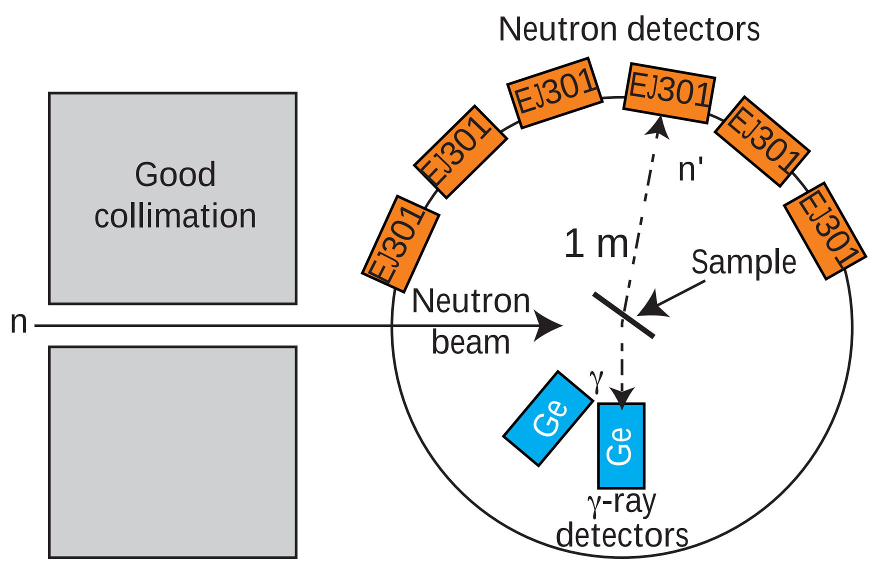
Following the great successes of GEANIE—a large array of high-resolution γ-ray detectors—we designed FIGARO for high-resolution detection of γ-rays from neutron-induced interactions with selected target nuclei, and we included the possibility of also detecting neutrons emitted in the reaction. With these neutron detectors, spectra of neutrons emitted in neutron-induced fission could also be measured.

The FIGARO layout is shown schematically in Fig. 1. Although FIGARO has fewer γ-rays detectors than GEANIE, it offers other features including

- many neutron detectors for the study of neutron-gamma coincidences;
- extremely good collimation of the incident-neutron beam for background reduction;
- a flexible experimental area to optimize detection efficiency and to allow for the evaluation of other detectors, such as fission chambers; and
- a PC-based data-acquisition system.

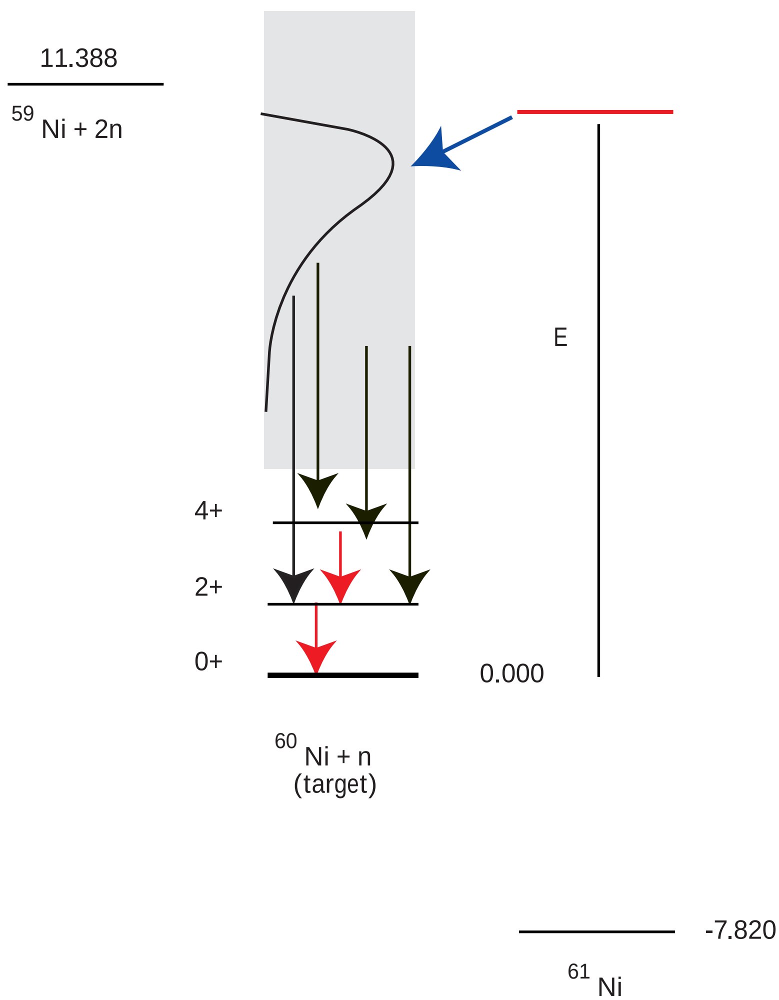
The use of FIGARO supplements that of GEANIE, which is oversubscribed.

The experimental approach with FIGARO is as follows: A pulse of neutrons having a wide energy spectrum is produced in the Target-4 spallation neutron source at WNR by the interaction of the 800-MeV proton beam from the LANSCE accelerator with a tungsten target.



↑ *Fig. 1.* *Schematic layout of FIGARO showing high-resolution γ-ray detectors and neutron detectors around the sample. In our commissioning experiments for the neutron detectors, the sample was replaced by a fission chamber, and the γ-ray detectors were removed.*

The neutrons, collimated to a beam of 1 to 2 cm in diameter, impinge on a sample 20 m from the source, where nuclear excitations take place. The excited nuclei decay by the emission of γ-rays, which are detected by high-resolution γ-ray detectors near the sample. The time of flight (TOF) of the incident neutrons gives the energy at which the reaction is initiated. The γ-ray energy indicates the particular level excited and consequently also the residual nucleus when there is more than one possible reaction (Fig. 2). Because the neutron pulses occur 35,000 times per second, we can accumulate many events to indicate the probability (cross section) of producing particular γ-rays as a function of incident-neutron energy.



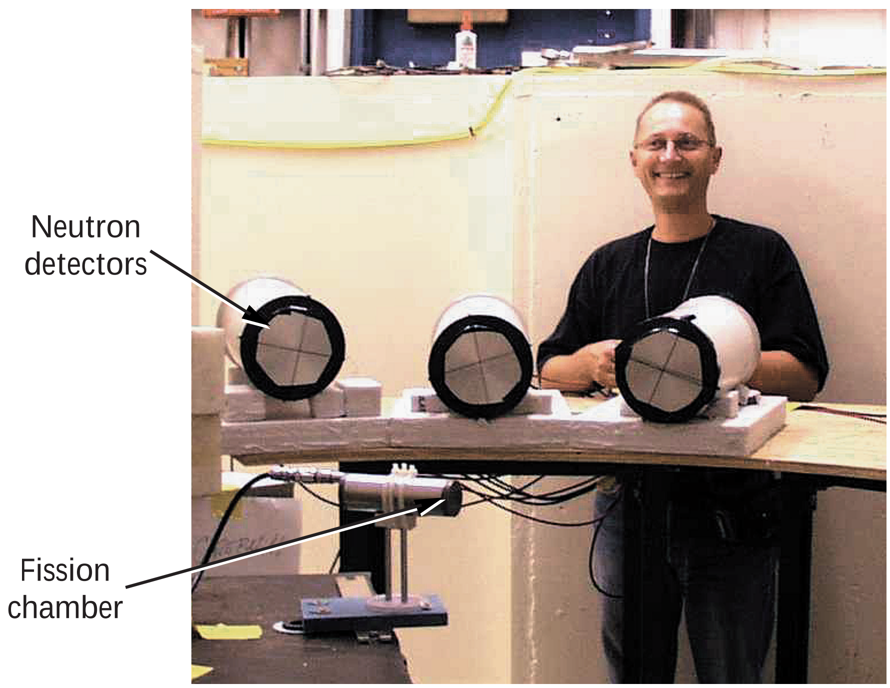
↑ ***Fig. 2.*** *In this simplified energy diagram, a fast neutron of energy En interacts with a ^{60}Ni nucleus, forming a compound, excited ^{61}Ni nucleus that decays by neutron emission. Neutrons are emitted and populate a range of excitation energies in ^{60}Ni according to optical-model transmission coefficients (which are fairly well known) and the density of excited levels (which is not well known). The energy of the emitted neutron specifies the excitation energy in ^{60}Ni, which decays by a γ-ray cascade to reach the low-lying states of known spin and parity. If the spin of the initial level in ^{60}Ni is high, then it will likely decay through the 4+ state. On the other hand, if the spin is low, the γ-ray cascade will likely bypass the 4+ state. Thus, the relative intensities of 4+ → 2+ and 2+ → 0+ transitions, which we detect, give information on the spin of the states in ^{60}Ni populated by neutron emission. The intensities of these two transitions reflect both the nuclear level density and the probability of a neutron being emitted from ^{61}Ni with certain ranges of angular momentum.*

Our first measurements were made with various nuclei (^{59}Co, ^{58,60}Ni, ^{99}Tc, ^{181}Ta, and ^{197}Au) to test nuclear-reaction models. These model calculations are subjected to stringent tests from measurements of the γ-rays produced in the various reactions. Because we already know the quantum numbers (spins and parities) of the residual states, comparing the measured cross sections to calculations tells us if angular momentum is being well handled by the calculations.

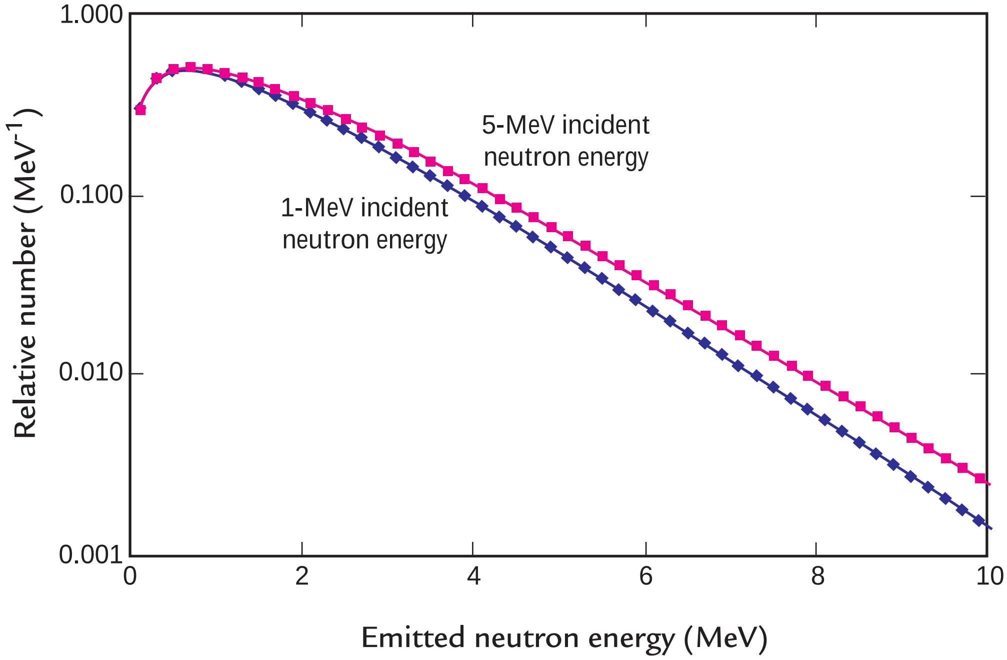
In 2001, we have added six neutron detectors to FIGARO at about 1 m from the sample so that the TOF of the emitted neutron (the "n'" in Fig. 1) can be measured and its energy deduced. By knowing the energies of both the incident and emitted neutron energies in an (n,n') excitation, we can ascertain the excitation energy of the nucleus. We can then investigate how the yield of a particular γ-ray depends on this excitation energy. Modern theories claim that certain excitation energies emphasize some angular momenta more than others do, and the distribution of angular momenta should be reflected in the γ-ray decay of low-lying levels where the angular momenta are known (see Fig. 2).

FIGARO Neutron Detectors Yield Data on Fission Neutron Spectra

To commission the neutron detectors and demonstrate that TOF can be measured over this 1-m distance from the sample, we substituted a ^{238}U fission chamber (provided by the French CEA-Bruyères-le-Châtel Laboratory) for the "sample." In this case, we did not use the γ-ray detectors at all, but used the fission chamber signal as the "start" signal for the TOF of fission neutrons. The apparatus is pictured in Fig. 3, showing three of the six neutron detectors (the remaining three detectors are positioned at other angles). We expect to see a change in shape of the fission-neutron spectrum as a function of the incident-neutron energy (Fig. 4). This effect has already been seen at discrete incident-neutron energies, but the FIGARO measurement is the first to our knowledge where a continuous-in-energy ("white") incident-neutron source has been used. Thus for the first time we can trace out the changes in shape of the fission-neutron spectrum with incident-neutron energies from 1 MeV to over 100 MeV. Knowledge of the shape of the fission-neutron spectrum is important in interpreting



↑ ***Fig. 3.*** *FIGARO as configured to measure fission-neutron spectra. Only three of the six neutron detectors are shown. The neutron beam enters from the left and passes through the fission chamber. A signal is generated by the fission chamber and serves as a trigger and "start" signal. Neutrons are detected by the neutron detectors, and their signals serve as "stop" signals. The TOF from the fission chamber to the neutron detectors is the difference in time between the start and stop signals, and the emitted neutron energy is determined directly from this flight time. The TOF of the incident neutron from the neutron source (20 m to the left in this picture) to the fission chamber gives the energy of the incident neutron. Thus, this is a "double TOF" experiment.*



↑ ***Fig. 4.*** *Schematic of fission-neutron-energy spectra whose shape is expected to change with the energy of the incident neutron. The expected neutron-emission spectra for two different incident neutron energies are shown.*

weapons test data, in calculating nuclear criticality, and in obtaining a better understanding of the fission process.

Future Development

Based on the positive results with the present FIGARO array of detectors, we plan to increase the number of neutron detectors to improve the efficiency of fission-neutron and gamma-neutron coincidences. With fission chambers in the beam, we will measure the fission-neutron spectra from neutron-induced fission of ^{235}U and ^{239}Pu with our CEA coworkers. With the improved gamma-neutron coincidence efficiency, we will be able to study nuclear-level densities over a wide range of nuclei, including closed-shell, rotational, and fission-product nuclides.

Asterix

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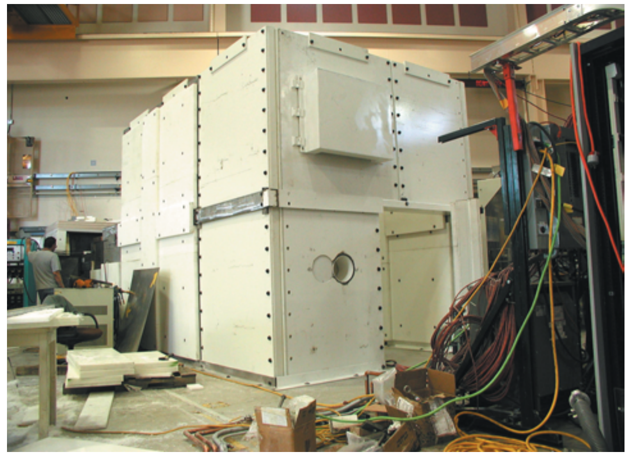
The goal of the Asterix project is to produce a highly polarized intense beam of cold neutrons that has a very large cross section (2 x 12 cm^2) and covers a wide wavelength range—and to do so while minimizing the fraction of the neutron beam that is not used. The project achieves its goal by embedding polarizing transmission supermirrors inside a nickel-coated neutron guide. The neutron guide is used in lieu of mechanical slits. When properly arranged within the guide, the supermirrors produce a polarized neutron beam with divergence that scales with wavelength. Thus, neutrons of all wavelengths are efficiently polarized. (In contrast, a neutron beam passing through mechanical slits has fixed divergence; consequently, long-wavelength neutrons are lost at the expense of polarizing short-wavelength neutrons.) Crucial to the success of this project was the acquisition of high-quality polarizing transmission supermirrors.



↑ ***Fig. 1.*** *Photograph of the new Asterix spectrometer cave. The use of non-magnetic materials in the cave's construction is essential for operation of the 11-T superconducting magnet. The cave's size (particularly its height) is required to accommodate tall sample-environment equipment, such as the 11-T magnet and the ILL "orange" cryostat.*

The Asterix spectrometer enables researchers to pursue investigations of non-uniformity in magnetic (or electronic) heterostructures (i.e., induced, or coerced, magnetization at or near interfaces). In addition to studies of nanostructured materials, research involving magnetically ordered novel bulk materials—for example, diffraction measurements of materials in very high magnetic fields using cold neutrons—is also possible.

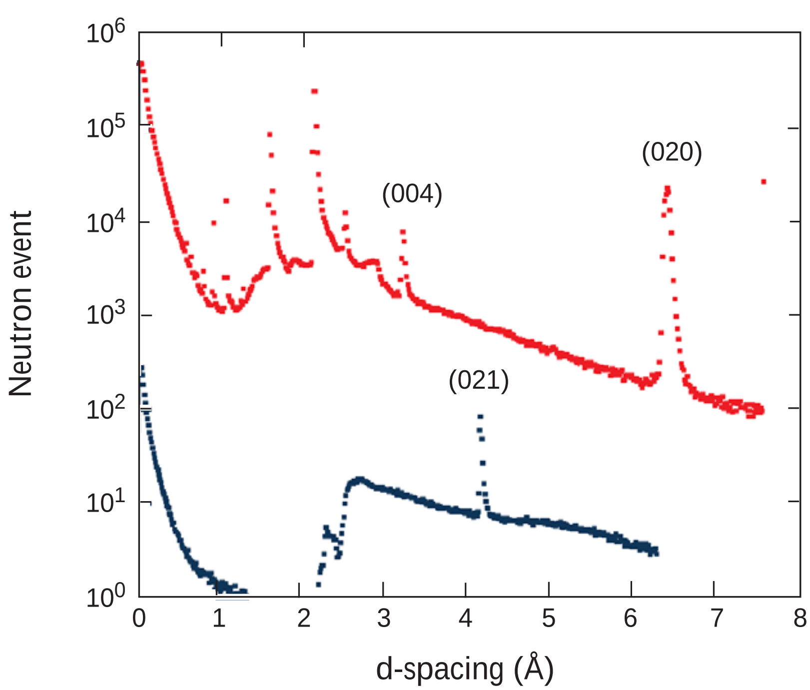
Recently, the experimental cave on flight path 11, which was formerly used by the nuclear-physics program, was replaced with a larger cave made from primarily non-magnetic materials (Fig. 1). This new construction enables studies that (1) use world-class sample-environment systems, such as the 11-T superconducting magnet (Fig. 2), the Institute Laue Langevin (ILL) "orange" cryostat, the Stishov high-pressure cell, and the cryostat furnace, and (2) take advantage of Asterix's high-intensity, polarized-cold-neutron beam. An unpolarized-neutron-beam option is also available. Because the Asterix spectrometer was constructed to serve a diverse magnetic/electronic-material community, it includes small-angle and wide-angle neutron-detection capabilities with polarization analysis as desired.

↑ ***Fig. 2.*** *Photograph of the new LANSCE 11-T superconducting magnet. The neutron shielding for Asterix was designed so as not to interfere with the operation of the magnet. The magnet was tested at LANSCE in December 2001 and achieved our specifications for maximum field in symmetric and asymmetric modes of operation.*

Asterix Activities Conducted in 2001

During the 2001 Asterix run cycle at Lujan Center, we achieved a number of key accomplishments, as discussed below.

Measurement of the order parameter of $LaSrFeO_4$ with unpolarized neutrons. During the first week of beam in 2001, we made an important measurement demonstrating the capability of Asterix to obtain wide-angle diffraction patterns from small samples in record times. Specifically, we studied a 2 x 2 x 1 mm^3 $LaSrFeO_4$ sample. The intensity measured, using just one tube in the position-sensitive detector array, as a function of d-spacing is shown in Fig. 3 for two sample orientations. In the upper curve, several nuclear Bragg reflections are observed. Nearly 150,000 neutron events were recorded during a 16-hour run in the (020) Bragg reflection. We compared the results obtained from Asterix to those taken for the same sample on the Single-Crystal Diffractometer (SCD). For the large d-spacing reflections relevant to studies of magnetism and complex materials comprising large unit cells, Asterix outperformed the SCD by more than a factor of 500. The lower curve shows the (021) Bragg reflection that is purely magnetic in origin (due to the antiferromagnetic order in $LaSrFeO_4$).



↑ ***Fig. 3.*** *Intensity measured as a function of d-spacing for two orientations of an $LaSrFeO_4$ sample. The intensity of the (021) reflection was measured as a function of temperature from 10 K to 350 K, producing the first determination of the order parameter for this complex material.*

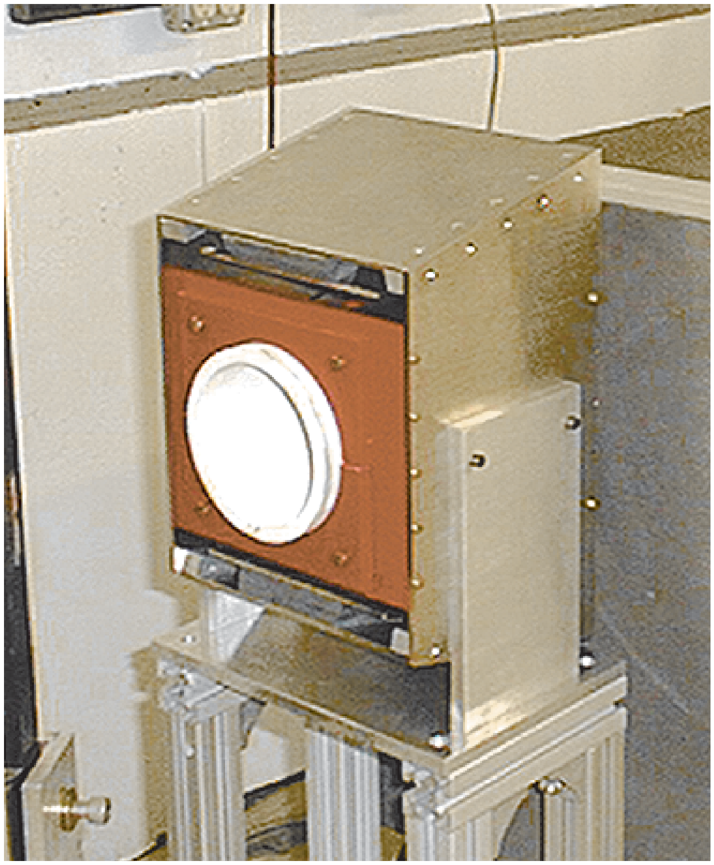
This demonstration is important in that it shows that even with the 30-T pulsed magnet operating at a frequency of 1 Hz (thus, only 1 in 20 neutron pulses provides useful information), there is still sufficient neutron flux to observe large d-spacing Bragg reflections. For example, we anticipate that typical experiments using this magnet will require roughly 12 hours of beam time (equivalent to 0.4% of the magnet's lifetime). (A prototype of the 30-T pulsed magnet is under construction at the National High Magnetic Field Laboratory.) The high flux of Asterix will not only be important to the pulsed-magnet program but will also enable studies of very small samples—that is, samples that might be small due to their actinide content or the availability of neutron isotopes.

Commissioning of polarized-neutron-beam optics. We demonstrated effective extraction of a polarized neutron beam through the novel polarization cavity. The beam polarization was typically 93% to 94% over the entire wavelength band. A higher polarization is desirable. During the 2002 run cycle, new polarizing supermirrors will be installed, and we anticipate achieving a polarization of 96%.

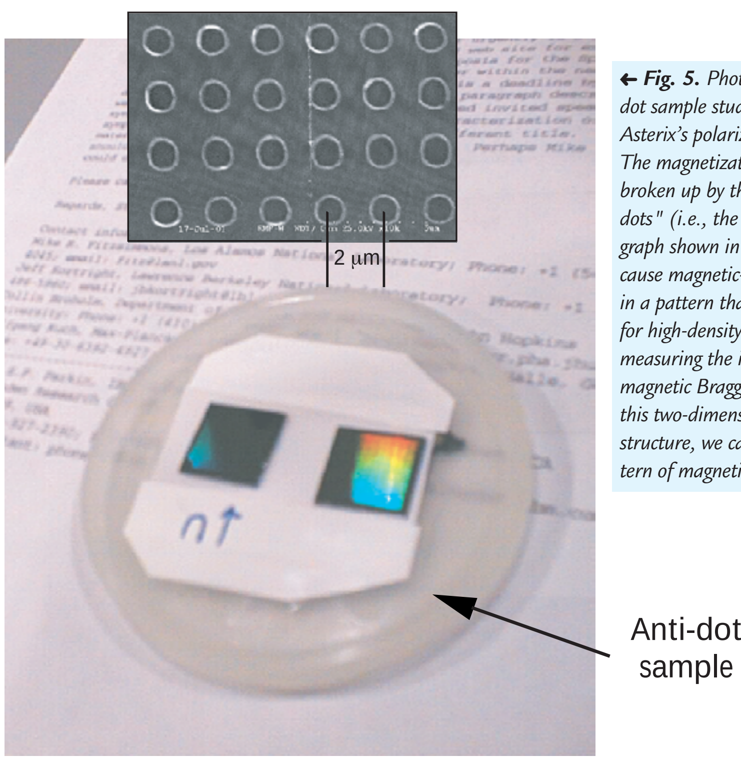
We also demonstrated nearly 99% efficient flipping of the polarized-neutron beam using a magnetic-field-gradient-radio-frequency (∇HRF) spin flipper (Fig. 4). These spin flippers exceeded our most optimistic goals. Unlike other radio-frequency spin-flipper technologies, the ∇HRF spin flipper does not exhibit decay in flipping efficiency with neutron wavelength, and flipping is achieved without the need to place materials in the neutron beam. Thus, the ∇HRF spin flipper is compatible with Asterix's unpolarized-neutron-beam operation mode.

Data collection using polarized neutrons. To demonstrate our success with development of Asterix's polarized-neutron-beam capability, we performed four neutron-scattering experiments. These experiments involved studies of

- magnetization-reversal mechanisms in exchange-biased systems with thin and thick ferromagnetic iron films,

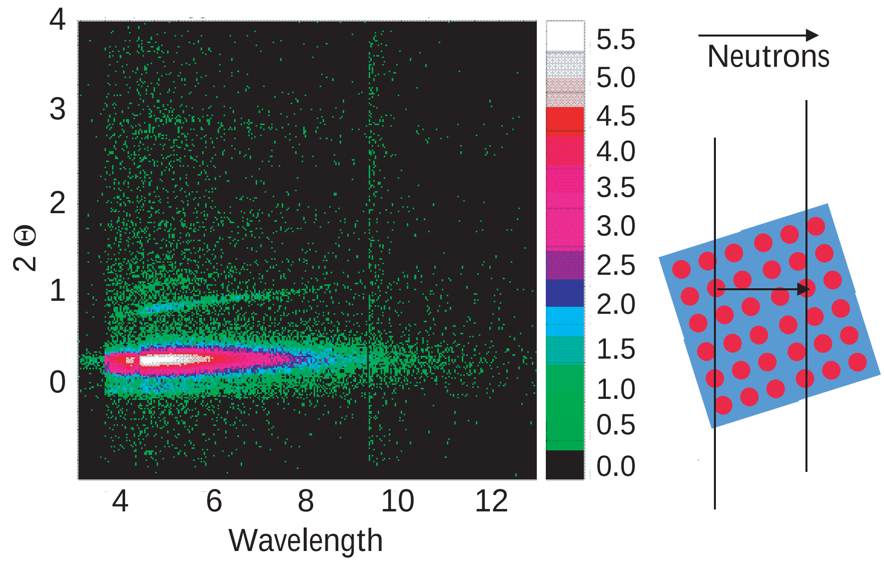


↑ ***Fig. 4.*** *View of the* ▽HRF *spin flipper.*



← ***Fig. 5.*** *Photograph of the anti-dot sample studied in 2001 with Asterix's polarized neutron beam. The magnetization of the film is broken up by the holes, or "anti-dots" (i.e., the electron micrograph shown in the inset), which cause magnetic-domain formation in a pattern that may be suitable for high-density data storage. By measuring the intensities of the magnetic Bragg reflections from this two-dimensional periodic structure, we can obtain the pattern of magnetization.*

- magnetization-domain formation in next-generation magnetic-recording media with perpendicular anisotropy,
- magnetic properties of 1.4-nm-thick iron oxide layers buried in iron, and
- magnetization of an array of anti-dots (holes) in a cobalt film.



↑ ***Fig. 6.*** *An intensity plot of a Bragg reflection from the anti-dot sample measured with polarized neutrons and using polarization analysis.*

The array of anti-dots studied consisted of 26 million, 1-µm-diam holes arranged in a square array (lattice parameter equal to 2 µm) (Fig. 5). Remarkably, we succeeded in measuring several Bragg reflections from this sample using polarized neutrons and polarization analysis. One example of such a measurement is shown in Fig. 6. The intensities of the reflections in the non-spin flip and spin-flip channels will be compared to those from micromagnetic calculations of the square array to test our theoretical understanding of how the formation of magnetic domains occurs when the domain size approaches length scales in patterned media.

Development of High-Performance Cold-Neutron Spectroscopy at LANSCE

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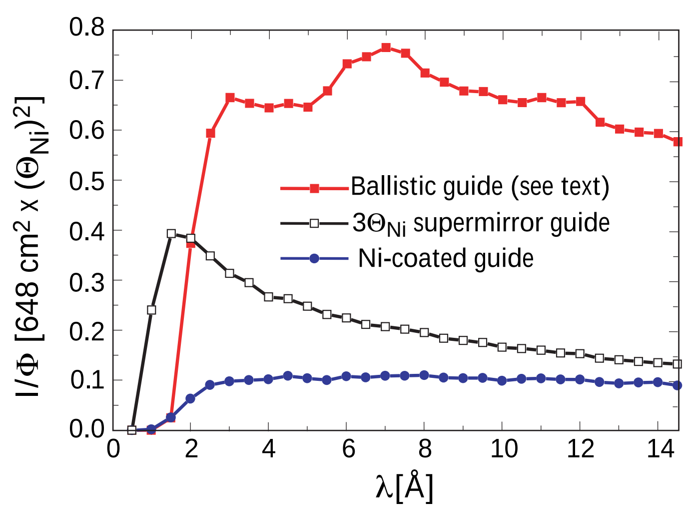
This research, called the "IN500 project," aims at developing novel techniques for achieving unprecedented sensitivity (neutron count rate) in cold-neutron spectroscopy. It will allow the exploration of microscopic and nanoscale dynamics in a variety of condensed-matter systems whose past study was hampered by low counting rates. A particularly important example is the study of collective dynamics in non-single-crystalline samples, where one cannot take advantage of the periodic nature of the reciprocal space to enhance the dynamic signal by working in higher Brillouin zones. Indeed, the tendency of the dynamic structure factor to scale with Q^2 makes the signal vanishingly small for small momentum transfers Q corresponding to distances beyond first nearest atomic neighbors in noncrystalline matter. The new capability will allow us to study nanoscale dynamic correlations in variety of complex matter systems, such as polymer melts, glassy systems, biopolymers, nanostructured matter, etc. To achieve this goal, three innovative approaches, discussed below, will be combined to gain a factor of 30 in neutron sensitivity compared to the most powerful spectrometer, IN5 at the Institut Laue Langevin (ILL), now available for this kind of research. (Note that IN5 has been rebuilt following ideas similar to one component of the IN500 project and a sensitivity gain of about a factor of 8 to 9 is expected when it returns to operation).

Combined Techniques

The three innovative techniques combined in the IN500 approach are: (1) the use of a high-intensity coupled moderator, (2) an enhanced beam extraction and delivery to the sample by a supermirror ballistic neutron guide, and (3) a repetition-rate multiplying chopper system. These techniques, which are unique to the Los Alamos Neutron Science Center (LANSCE) for the time being, are already included in the plans of future spallation sources such as the Spallation Neutron Source and the European Spallation Source. Pioneering work at Los Alamos National Laboratory (LANL) will also help to efficiently implement these new techniques at these future facilities.

Coupled moderators were first developed and implemented on a pulsed spallation source at the Lujan Neutron Scattering Center (Lujan Center) in 1998. The coupled cold (liquid H_2) moderator used in the IN500 project on flight path (FP) 13 is expected to offer about four times the brightness of conventional cold moderators used at the Lujan Center by now and at the Rutherford-Appleton Laboratory Neutron Facility (ISIS), the current premier spallation source. The coupled cold moderator at the Lujan Center provides the highest peak cold-neutron flux ever achieved: about three times superior to that of the ILL high-flux reactor. This gain of brightness is inevitably related to an extended pulse length, with significant neutron intensity emitted by the moderator up to 3 to 4 ms after the sharp rising edge of the pulse. One of our challenges will be to establish the efficient use of such enhanced intensity pulses in neutron spectroscopy by new techniques to eliminate the detrimental effects of the long tails on resolution and background. The new, coupled cold moderators at the Lujan Center had previously not been accessible to beam lines. Vacuum jackets to house the beam-extraction supermirror guides were successfully installed in early 2001 on FP13 and FP12. The design, fabrication, and installation of the beam shutter and surrounding shielding has been completed. We will perform the first experimental characterization of the new cold moderator in fall 2002.

For enhanced beam extraction and beam transport, a supermirror-based "ballistic-guide" prototype has been designed and optimized by Monte Carlo simulations (Fig.1). This guide system will deliver—with some 30%



↑ ***Fig. 1.*** *Efficiency of neutron-beam delivery by the IN500 ballistic guide as a function of neutron wavelength (simulation results) in comparison to conventional, uniform supermirror and Ni guides.*

loss of flux only—beam to the sample corresponding to the neutron intensity in a 162-cm^2 cross-section conventional Ni-coated guide, compressed into a 20.4-cm^2 downstream guide exit window at 62.5 m from the moderator. In comparison, the old IN5 instrument at the ILL used 13-cm^2 worth of Ni-guide flux, and the new one will achieve 60 cm^2.

The third IN500 technique involves the use of repetition rate multiplication (RRM) to enhance the efficiency of pulsed neutron sources in general in inelastic spectroscopy. The time needed for neutron time-of-flight analysis over the typically 3- to 6-m distance between the sample and the detector is about 2 to 10 ms, i.e., the process could be repeated 100 to 500 times per second. In contrast, pulsed spallation sources, existing or planned, only deliver 10 to 60 source pulses per second, and by the conventional approach the spectrometer is idle for 50% to 90% of the time between subsequent source pulses. Using RRM, a complex chopper system selects from each source pulse a set of monochromatic neutron beams with different wavelengths, which arrive at the sample as distinct pulses and are separated one from the other by a time interval defined by the chopper settings. On IN500, in contrast to the 50-ms time between subsequent source pulses, the time between subsequent chopper pulses on the sample will be between 4.17 and 25 ms, freely chosen for the needs of the experiments.

During 2001, we completed the design and numerical simulation of the RRM chopper systems and placed the order for its fabrication. The system consists of six disc choppers, each 700-mm in diameter and rotating with speeds ranging from 1,200 to 15,000 rpm. Two of the choppers consist of a pair of counter-rotating discs. The timing of the chopper pulses, relative to each other, will be precise to within 0.1 μs. The chopper system also accomplishes the functions of sharply cutting the trailing edge of the source pulses by which the resolution can also be adjusted. The large variety of functions that the system will control dictates the need for eight independently controlled discs for pulse shaping; pulse-tail cutting; the selection of up to twelve monochromatic pulses with different wavelengths from each source pulse; and, most importantly, making sure that no undesired, parasitic pulses filter through the system.

The large gain in sensitivity compared to reactor instruments comes from the first two innovations: (1) higher peak flux due to the high-intensity moderator and (2) enhanced beam delivery by an advanced neutron-guide design. In this respect, the third innovation, RRM, only eliminates the drawback of the common instrument-design principle on pulsed sources of tying the pulse frequency on the sample to that of the source.

Conclusion

The IN500 project is on track for completing the operational tests of the prototype ballistic guide and RRM chopper system on a high-intensity coupled moderator by September 2003. With the new techniques established and with the addition of a state-of-the-art detector chamber with a 3-m radius and about 10-m^2 detector area coverage, IN500 would provide experimenters with a most powerful low-energy neutron spectrometer.

Protein Crystallography Station—Commissioned and Ready for Users

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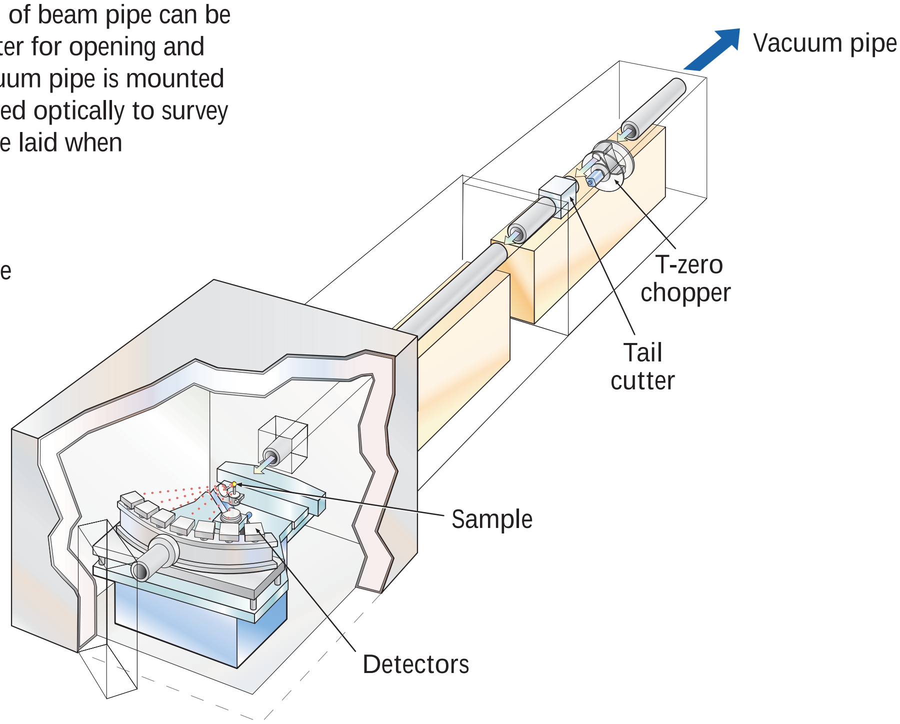
The new neutron Protein Crystallography Station (PCS)[1] located at the Los Alamos Neutron Science Center (LANSCE) was declared "ready for beam" in December 2000. In 2001, the PCS was fully commissioned by B Division with support from LANSCE. The PCS, which is funded by the Department of Energy Office of Biological and Environmental Research, will become part of the LANSCE User Program in 2002. The PCS is located at the Lujan Neutron Scattering Center (Lujan Center) on flight path 15, viewing a coupled water moderator where neutrons are emitted in pulses at a rate of 20 or 30 Hz.

System Development and Installation

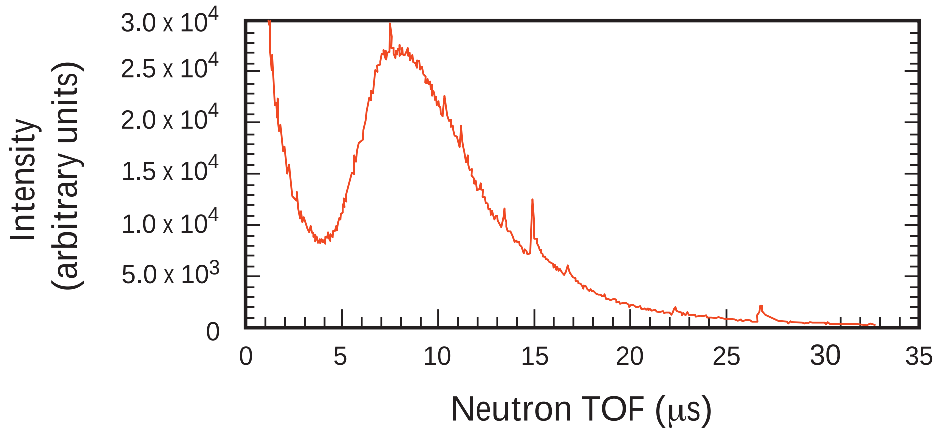
The neutron beam transport system and shielding were installed before the end of the 2000 LANSCE run cycle. The neutron beam transport system consists of about 28 m of vacuum pipe between the neutron source and the sample position as shown in Fig. 1. The vacuum pipe carries the neutrons out of experimental area ER-1 through a wall into ER-2 and has collimation inserts that taper the incident neutrons to produce a fine, almost parallel beam that hits the crystal sample. These inserts extend back into bulk shielding that surrounds the moderator where a 2-m section of beam pipe can be filled with mercury to act as a shutter for opening and closing the neutron beam. The vacuum pipe is mounted on adjustable stands and was aligned optically to survey monuments (cross marks) that were laid when the mercury shutter was installed in the bulk shield in 1999.

A shielding of iron and polyethylene laminate was installed around the vacuum pipe in ER-1 with provisions for a cavity for the future installation of a chopper. A magnetite concrete and polyethylene shield was installed around the vacuum pipe in ER-2. The shielding opens up to a large cave at the sample position in ER-2. This cave was installed as interlocking monolithic blocks that were bolted together. After the shutter and personal access control systems were installed and tested and after a background radiation survey was completed, the station was declared "ready for beam" with two weeks of beam time left in the 2000 run cycle.

Receiving first beam at the end of the 2000 run cycle was a tremendous achievement for which the installation team (LANSCE-7) and the ER-1 shielding designer (Kathy Lovell, LANSCE-12) received Distinquished Performance Awards (see related stories on p. 182). These two weeks of beam time proved to be extremely important. In our first experiment, line shapes of 9 orders of diffraction data were collected from a fluorophlogopite crystal to characterize, for the first time, the neutron time dispersion of the coupled water moderator (Fig. 2).[2] The results indicate that the "coupling" of the spallation neutrons to the moderator is smaller than projected, implying a shortfall in neutron flux but a better time resolution. Because the measured, integrated neutron flux of the direct beam at the sample position was a factor of 40 below projections, the neutron beam transport system was judged to be neutronically misaligned.



↑ ***Fig. 1.*** *Protein Crystallography Station beam layout.*



↑ ***Fig. 2.*** *A time-of-flight (TOF) diffraction pattern from a fluorophlogopite crystal. The various Bragg peaks correspond to wavelengths ranging approximately from 1 Å to 4 Å.*

Data were successfully collected from a Vd-Nb sample using a small 200-mm x 200-mm position-sensitive detector provided by Brookhaven National Laboratory (BNL) and an initial VME (virtual memory extension) single-crate version of the data-acquisition system (DAQ).

Beam Realignment

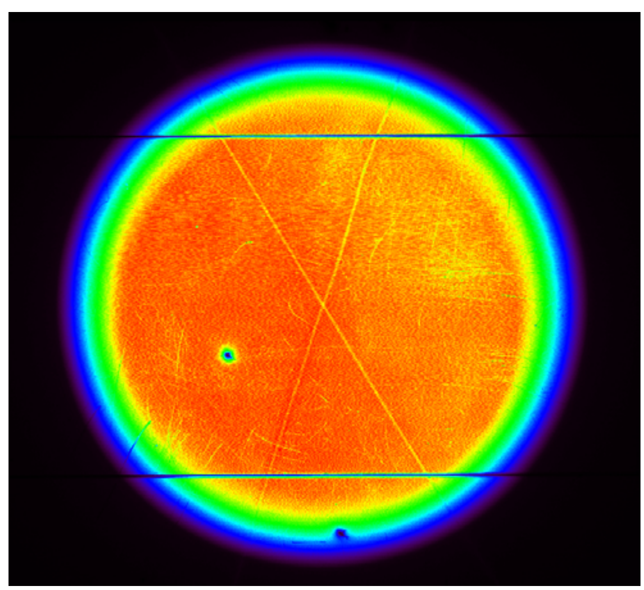
During the scheduled outage in 2001, the shielding was disassembled and the optical alignment of the neutron beam transport system was found to be consistent with the survey monuments. When neutrons became available again in June 2001, the easily accessible part of the vacuum pipe was realigned to follow the peak in the distribution of the neutron beam flux. We determined this distribution by placing neutron-image-plate detectors and pinhole collimators at various positions along the beam line (Fig. 3). This alignment of the neutron beam differed by 0.01° from the optical alignment and improved the direct-beam-integrated neutron beam flux at the sample position by more than a factor of 10. The neutron beam flux remains a factor of 3 to 4 smaller than projected, and we are still investigating whether this finding is due to moderator performance or beam misalignment before the chopper cavity.

Final Installations

During August 2001, a team from BNL replaced the small detector and its electronics with a larger 120° x 16° detection system. Shortly after installation, a number of small problems with the detector and its communication with the DAQ were identified and have since been rectified. The detector and a VME multi-crate version of the DAQ were commissioned, and an instrument control system was developed and installed. The instrument control system controls the sample and detector goniometer motors and interfaces with the DAQ to coordinate data collection with motor movements. A graphical user interface, which is unique to PCS, provides a user-friendly means of conducting experiments. The station was finally ready for commissioning experiments after the chopper was successfully installed and tested in ER-1 by September 2001.

Commissioning Experiments

Commissioning experiments were chosen to test various aspects of the PCS. Single crystals of myoglobin, cobalamine (II), and α-glycine were used to probe the diffraction resolution of the PCS and also to provide data



↑ ***Fig. 3.*** *A neutron-image-plate recording of the neutron beam flux. The image plate was placed at a break in the vacuum beam pipe, 11 m from the moderator, with cross wires marking the center of the vacuum pipe. The recorded neutron flux increases from blue to red. This image shows that the beam has a circular profile and is fairly homogeneous.*

sets for testing the data-analysis software. Myoglobin is an oxygen-transport protein with a relatively large unit cell that diffracts neutrons to about a 2-Å resolution. Cobalamine (II) is a reduced form of the vitamin B12 coenzyme, and α-glycine is an amino acid and neurotransmitter. Both have smaller unit cells and diffract neutrons to atomic resolution. Complete data sets were collected from all three systems. Data were collected well beyond the projected 1.5-Å resolution limit of PCS (Fig. 4). To test the performance of the PCS for fibrous samples, we also collected complete data sets from the polysaccharide cellulose Iβ, which was extracted from the mantles of *Halocynthia roretzi*,[3] and from calf thymus DNA.

In the final two weeks of the 2001 run cycle, we tested the feasibility of future experiments with samples supplied by users. These samples included single crystals of insulin grown for microgravity experiments in space;[4] the photosynthetic reaction center (PRC) of *Rhodobacter sphaeroides*, which is a large membrane-bound protein complex responsible for converting photons of light into chemical energy;[5] and oligonucleotide d(CGCGCG), which is a short synthetic fragment of DNA. The most striking results were obtained with the PRC of *Rhodobacter sphaeroides*, whereby a crystal was placed in the beam for about a fifth of the normal exposure duration with a reduced proton beam delivery of 48 μA rather than at the 200-μA design specification. The

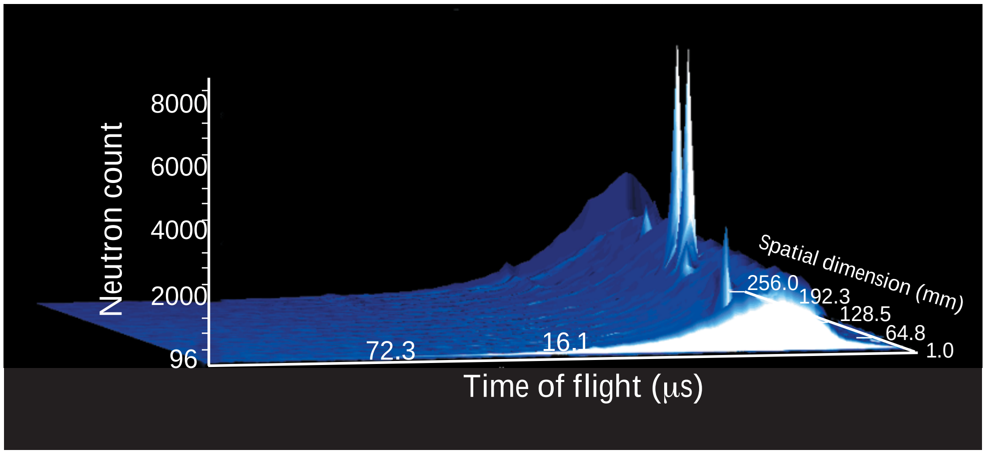


Fig. 4. *Diffraction data collected from cobalamine (II) in a small area of the detector. The data, which were collected in two spatial dimensions and one time dimension, have been summed along one of the spatial dimensions so that it can be represented as an isometric view with the TOF axis in the horizontal position and the remaining spatial axis pointing into the page. The slowly varying background scattering is due mostly to unwanted incoherent scattering from hydrogen and reflects the distribution of neutron wavelengths in the incident-beam spectrum. The sharp peaks that sit on the background are the desired Bragg diffraction peaks from the crystal.*

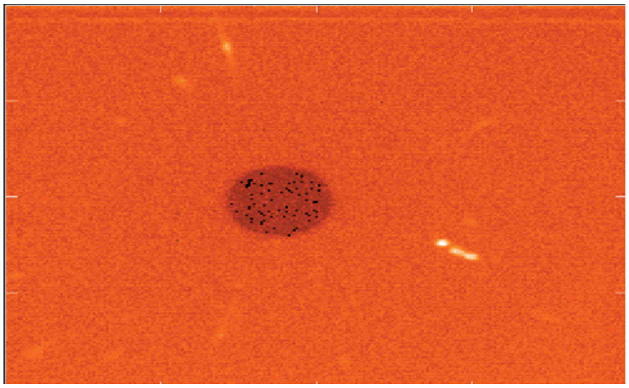


Fig. 5. *Image from a small area of the detector showing diffraction data collected from crystals of the PRC of Rhodobacter sphaeroides. The data have been summed along the time dimension so that it can be represented in its two spatial dimensions. The light spots in these images correspond to Bragg diffraction peaks from the crystals. The large dark spot near the center of the image is a shadow of a beam stop placed in front of the detector.*

crystal had a volume below the lower end of the design feasibility range for the PCS (< 1 mm^3) and a unit-cell volume three times larger than the upper end of the design feasibility range for the PCS (i.e., 1 x 10^6 $Å^3$). Despite these circumstances, diffraction data (collected to < 5-Å resolution) indicate that under normal operations data taken at much higher resolution could be collected on the PCS from this large protein complex (Fig. 5).

Conclusion

The PCS has been commissioned and is ready to become part of the LANSCE User Program in 2002. Experiments carried out during the commissioning period are encouraging and indicate that the PCS will become a world-class, state-of-the-art instrument for structural biology.

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2. Measurements courtesy of L. Daemen, LANSCE-12.
3. Sample provided by Y. Nishiyama, Tokyo University.
4. Sample provided by R. Blessings, State University of New York.
5. Sample provided by M. Yousef, P. Thiyagarajan, and P. Laible, Argonne National Laboratory.

SMARTS—A New Spectrometer for Studies of Engineering Materials

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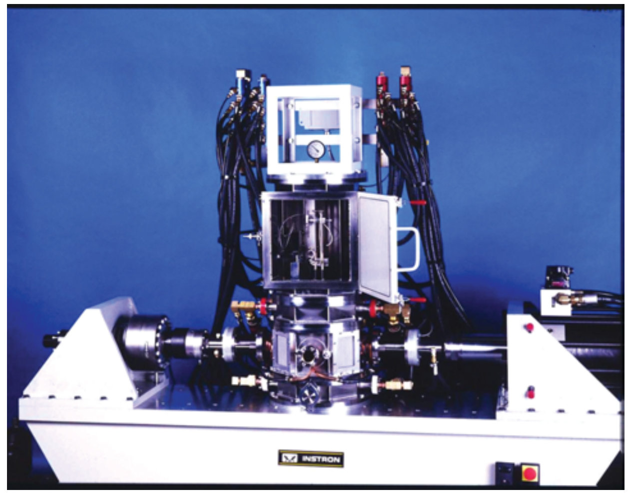
The Spectrometer for Materials Research at Temperature and Stress (SMARTS), a new instrument that dramatically expands the application of neutron diffraction to studies of engineering problems, was commissioned in the summer of 2001. It was funded by Basic Energy Sciences (BES) and built to augment the successful research program on the existing neutron powder diffractometer (which is currently being upgraded). SMARTS offers an extensive array of in situ capabilities. With a common theme of examining structural engineering materials, it has the flux to interrogate small (1-mm^3) specimens and the ease of access to accommodate large (1-m^3) samples. Components with dimensions up to 1 m and up to 1500 kg can be positioned precisely using a translator custom designed and recessed in the floor of experimental room ER-2 of the Lujan Neutron Scattering Center (to maximize the space underneath the beam). Alignment theodolites networked to a computer are located several meters from the specimen. Using commercial surveying software, they provide an efficient way to triangulate the position of objects in the beam to within 0.01 mm. Achieving this level of precision is critical for stress-strain measurements because misalignments of more than 0.1 mm can introduce systematic errors. Another piece of custom-designed equipment is a furnace and load-frame suite (Fig. 1) that enables research on materials subjected simultaneously to extreme loads and temperatures (18,000 kg and 1,500°C).



↑ Fig. 1. *The SMARTS load-frame and furnace suite.*

Progress in 2001

The shutter was opened for the first time on August 12, 2001, and by December 24 we collected 3,500 data sets. After calibration was completed, our approach to commissioning was to attempt an array of experiments that cover the range of expected activity. In doing so, we tested all aspects of the spectrometer and made a series of ergonomic improvements (i.e., relating to how experiments are performed and how data are processed) that will allow SMARTS to efficiently enter the BES User Program in the summer of 2002. By the end of the run cycle, approximately 15 different experiments were completed, many of which included collaborations with users from outside Los Alamos National Laboratory (LANL). The following LANL personnel were integral to the "on schedule" commissioning of SMARTS: T.A. Sisneros, T.M. Holden, B. Clausen, S.C. Vogel, J.J. Ross, G.M. Cooper, T. Kozlowski, R.B. Merl, and R.O. Nelson.

Following calibration runs using calcium fluoride, vanadium-niobium, and silicon single crystals, activity on SMARTS included the following experiments.

- Room-temperature loading in order of increasing stress on (1) Carrara marble at 150 MPa (T. Darling, LANL); (2) equi-channel processed aluminum at 180 MPa (S. Vogel, LANL); and (3) bulk-metallic-glass composites at 2,000 MPa (B. Clausen, California Institute of Technology).

- High-temperature loading in order of increasing temperature on (1) Al-Al_2O_3 at 200°C (J. Hanan and G. Swift, California Institute of Technology); (2) WC-Co at 900°C (D. Mari and K. Buss, Ecole Polytechnique Fédérale de Lausanne); (3) super-alloy CM 247 LC at 900°C (B. Majumdar, New Mexico Institute of Mining and Technology); (4) Waspaloy, an Ni-based superalloy at 950°C (D. Dye, National Research Council of Canada); and SiC Si_3N_4 at 1,400°C (Fig. 2) (C. Aydiner and B. Clausen, California Institute of Technology).

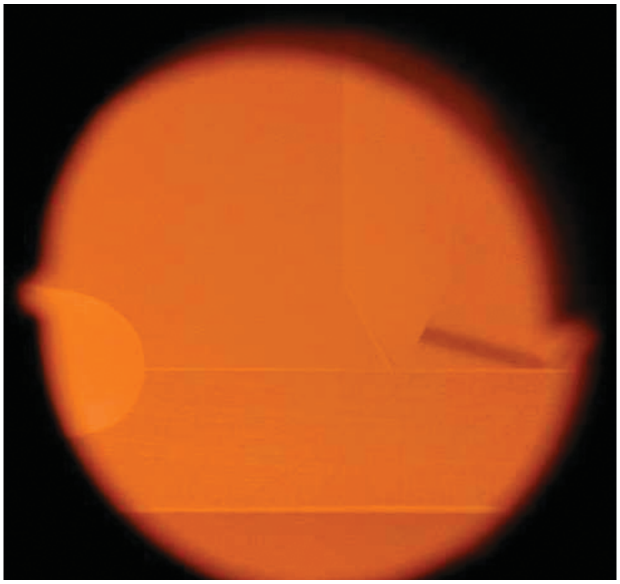


Fig. 2. *The furnace "hot zone" shown through a viewing port during the SiC Si_3N_4 measurements at 1,400°C.*

Fig. 3. *Steve Spooner (Oak Ridge National Laboratory) refrains from using theodolite-alignment technology during the measurements on a clad boiler tube, preferring to employ "old style" technology—a "ruler."*

- Spatially resolved measurements with sampling volumes between 8 and 20 mm^3 were performed on (1) a Haynes-25 weld for a satellite application (C. Larsen, University of Central Florida and Linköping University, and M. Stout, LANL); (2) a stainless-steel-clad, ferritic-steel boiler tube (Fig. 3) (A. Payzant, S. Spooner, and C. Hubbard, Oak Ridge National Laboratory); and (3) a classified problem (D. Brown, LANL).

- A high-pressure experiment was performed on NaOCN (K. Knorr, University of Kiel) and characterization runs were performed on a series of PZT (lead-zirconium-titanium oxide) specimens (R. Rogan, California Institute of Technology).

HIPPO—A New High-Intensity, Multiple-Environment Neutron Diffractometer

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The new time-of-flight (TOF) high-pressure-preferred-orientation (HIPPO) neutron diffractometer for materials studies has been completed and is now a part of the user program at the Lujan Neutron Scattering Center (Lujan Center). The majority of the HIPPO instrument was designed and manufactured at the Los Alamos Neutron Science Center (LANSCE) as part of the Short-Pulse Spallation Source Enhancement Project to upgrade LANSCE facilities as sponsored by the Department of Energy Offices of Basic Energy Science and Defense Programs. The HIPPO instrument is a combined effort between the University of California campuses and national laboratories to attain scientific excellence in neutron diffraction, to advance our present knowledge of condensed matter, and to make neutron diffractometry accessible to the national user community. HIPPO allows researchers and students to conduct real-time structural and textural studies in situ under a wide variety of environmental conditions, from low to high temperatures, at pressures up to ~ 30 GPa, and under stress. The high count rate achieved with HIPPO makes possible dynamic experiments that previously could not be envisioned with neutron diffraction—diffraction patterns can be obtained in minutes rather than hours. This unique neutron diffractometer supports a broad variety of disciplines, including materials science and engineering, earth sciences, physics, and chemistry. More than 100 users will be accommodated each year during an eight-month run cycle, and the easy and sustained access to HIPPO will encourage neutron-diffraction studies for graduate-student thesis research.

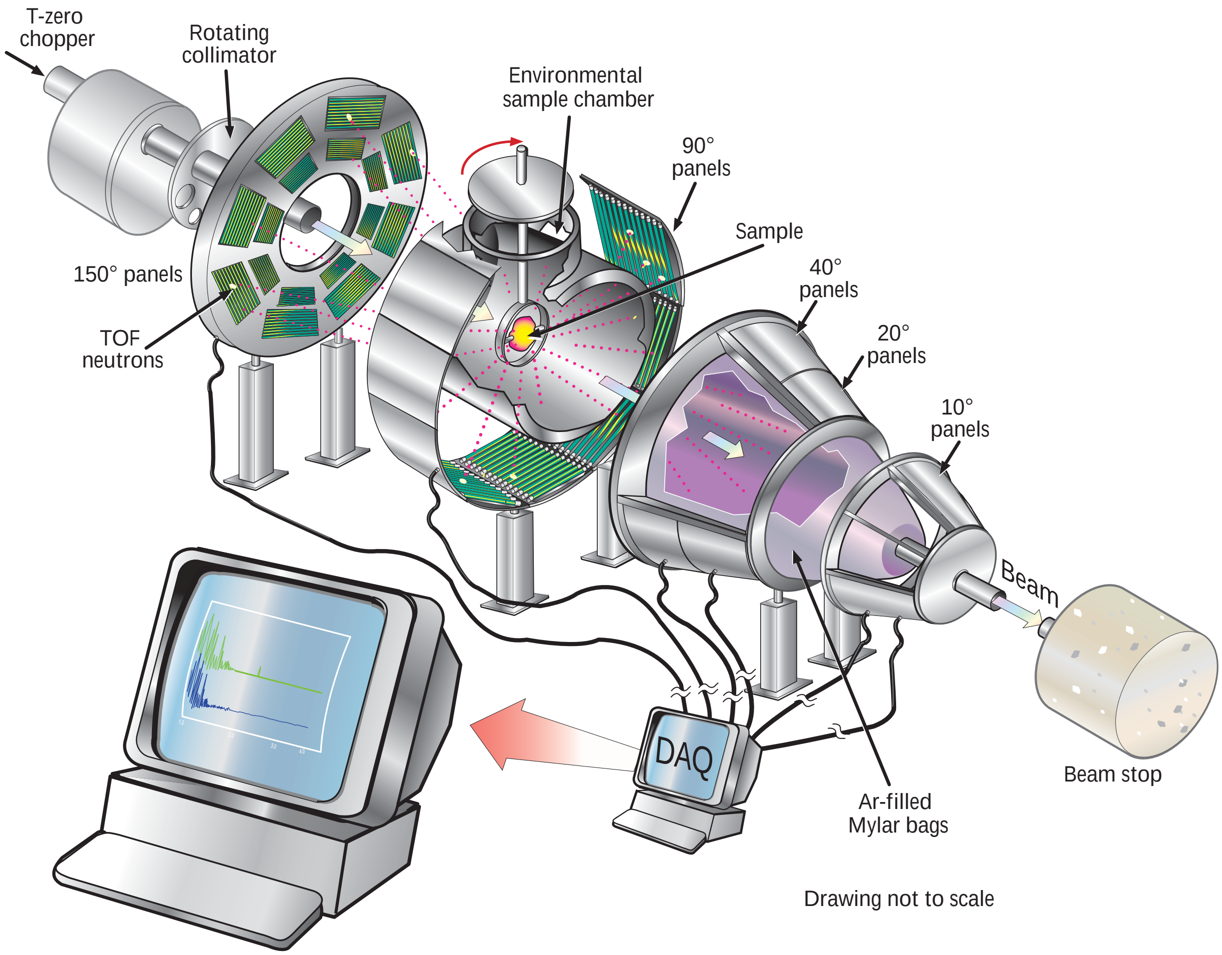
Advantages of Neutron Diffraction

Because neutrons can travel long distances through most materials without being significantly absorbed, they can be used to study atomic structures in bulk samples under a variety of experimental conditions. In addition, neutron diffraction provides information complementary to x-ray diffraction. For example, adjacent elements in the periodic chart often exhibit significant neutron-scattering contrast while being indistinguishable with x-rays, and light elements such as hydrogen and deuterium have large neutron-scattering cross sections. Important new neutron-diffraction applications have emerged in both applied and fundamental condensed-matter research as a result of the availability of new, high-flux instruments. Of particular interest to the research community is the investigation of small (1 mm^3) and large (2 cm^3) sample volumes at high (< 2,000 K) and low (> 10 K) temperatures, at high pressure (≤ 30 GPa), and in different atmospheres. In addition, the ability to measure neutron-diffraction patterns rapidly enables dynamic studies, previously done only on synchrotron sources. The high spectral resolution of HIPPO also allows the simultaneous determination of, for example, crystal structures, phase proportions, textures, and strains using modified Rietveld methods.[1,2]

A range of wavelengths is available for pulsed polychromatic neutrons, and continuous spectra can be recorded at moderate resolution. These types of neutrons are well suited for studying low-symmetry materials, composites with many diffraction peaks, and many environmental problems.[2,3] The textures of such complex materials typically cannot be satisfactorily characterized by x-ray diffraction. TOF neutron-diffraction techniques offer unique advantages over other methods in this area. Neutron-diffraction averages over large volumes rather than surfaces, making grain statistics for texture analysis easily obtainable. Also, because intensity corrections are generally unnecessary with this method, a high level of accuracy can be obtained.[4] The low-absorption property of neutrons allows researchers to use environmental stages (low and high temperature, high pressure, and bulk stress-strain) to observe *in situ* texture changes.[5,6] New crystallographic methods are being used to analyze these data to provide simultaneous information on crystal structure, orientation distribution, phase proportions, internal elastic strains (i.e., from peak locations), and microstructure (i.e., from peak shapes).[1, 2, 7]

State-of-the-Art Technology

Lujan Center's state-of-the-art target-moderator system produces pulsed thermal neutrons that travel down HIPPO's initial 9-m flight path (FP) (Fig. 1). A T_0 chopper removes the energetic neutrons produced at the neutron-production target, and a collimator guides the remaining beam toward the sample chamber.



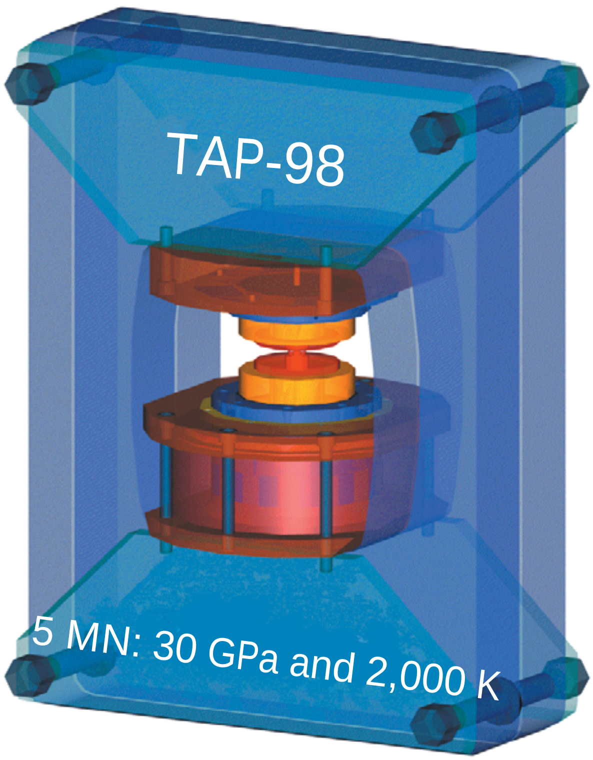
↑ ***Fig. 1.*** *Exploded view of HIPPO showing sample chamber surrounded by five conical three-dimensional rings of ^{3}He detector tubes at 10 atm. A white beam made up of pulsed neutrons of different energies (entering from the left) travels down a collimator to a chopper that eliminates very fast neutrons, allowing only slower thermal neutrons to continue down the FP to the bulk material contained inside a 29.13-in.-diam sample chamber. The neutrons interact with the crystal structure of the bulk material, diffract, and impinge on the detectors.*

Apertures gradually reduce the size of the beam as it travels toward the sample chamber and make it more coherent and focused. An array of 1,380 ^{3}He detector tubes covers nearly 4.6 m^2 with five detector banks at scattering angles ranging from backscattering (nominally 150°) to forward scattering (nominally 10°).

The new HIPPO diffractometer exploits the improved neutron source at LANSCE and a short FP to overcome a major limitation of neutron beams—their weak intensity. The count rate for some experiments is 20 times that currently obtained on the high-intensity powder diffractometer (HIPD) at the Lujan Center. It produces, within minutes rather than hours, TOF neutron-diffraction patterns from the combined output of its 1,380 ^{3}He-filled detector tubes.

Myriad Research Applications with HIPPO

HIPPO accommodates a wide variety of research requiring *in situ* neutron diffraction. A number of environmental stages are available, for example, a cryostat, a controlled-atmosphere 2,000-K furnace, a three-axis texture goniometer with Kappa geometry, a 100-kN stress rig, a sample changer, and a variety of high-pressure cells that include the new toroidal anvil press (TAP-98)[8] with its ability to reach 30 GPa and 2000 K (Fig. 2). VME-based (virtual memory extension) data acquisition makes use of Web-based visualization and control software. The ability to measure diffraction data rapidly using these environmental stages, coupled with Rietveld analysis, makes HIPPO the instrument of choice in areas of research, including phase transformations, high-pressure and high- and low-temperature



↑ ***Fig. 2.*** *The 500-metric-ton toroidal anvil press (TAP-98), which was custom designed for HIPPO by Yusheng Zhao (LANSCE Division), has sintered diamond anvils and is designed to expose a 5-mm-diam by 5-mm-long sample to 30 GPa and 2,000 K.*

studies, polycrystal anisotropy (texture), stress/strain, and complex materials crystallography. Researchers can study the dynamics of reactions, recrystallization, and deformation of bulk anisotropic properties under various temperature and pressure conditions. No other existing instrument has this capability.

HIPPO's three-dimensional arrangement of detectors allows researchers to make direct measurements of the orientation of crystals in polycrystalline samples using only very few sample rotations. An innovative sample changer holds 100 samples at a time for rapid powder-diffraction measurements and 32 samples at a time for rapid texture measurements.

In situ high-pressure-temperature (P-T) neutron-diffraction experiments provide a unique opportunity to study texture, hydrogen bonding, magnetic moments, and structural and thermal parameters of light and heavy elements, both of which are virtually impossible to study by x-ray diffraction. For example, we can derive thermoelasticities and Debye-Waller factors as functions of P and T using *in situ* high P-T neutron-diffraction techniques. These applications can also be extended to a much broader spectrum of scientific problems. For instance, puzzles in earth science, such as the carbon cycle and the role of hydrous minerals for water exchange between lithosphere and biosphere, can be directly addressed under geologically relevant P and T. Moreover, by introducing *in situ* shear strain, texture accompanied by phase transitions in the deep mantle can also be studied. The new TAP-98 press will accommodate *in situ* P-T neutron-diffraction experiments up to 30 GPa and 2,000 K simultaneously, using samples from 50 to 300 mm^3 in size. TAP-98 is normally positioned horizontally in the HIPPO sample chamber, and future plans include a vertical setting that would facilitate study of texture development and long-spacing diffraction lines.

Neutron scattering is also the primary tool for determining the spatial and temporal distributions of magnetization at the microscopic scale.[9] Magnetic scattering is due to an interaction between the magnetic moment of the neutron and the unpaired outer-shell electrons. Therefore, neutrons offer the unique capability to measure spin, charge, and lattice effects simultaneously. Most studies of magnetic scattering are effectively restricted to d-spacings greater than about 1 to 2 Å, but the HIPPO diffractometer covers significantly larger d-spacings. In addition, the large neutron flux of HIPPO will allow relatively fast measurements of magnetic materials, which often suffer from the fact that magnetic intensities are weak compared with nuclear-scattering intensities. Thus, magnetic systems can be thoroughly studied under a variety of P-T conditions using HIPPO.

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Upgrades to the Existing Experimental Area Personnel Access Control System

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This article describes the work performed in 2001 to install Experimental Area Personnel Access Control Systems (EPACS) at the Lujan Neutron Scattering Center (Lujan Center), the Weapons Neutron Research Facility (WNR), and the new Irradiation of Chips and Electronics Facility (known as the ICE House). There were no new Personnel Access Control Systems installed during 2001.

Lujan Center Installation Projects

During 2001, four new instruments (SMARTS, HIPPO, DANCE, and PCS) in experimental areas ER-1 and -2 at the Lujan Center were fitted with a new mercury shutter and an EPACS (Fig. 1). (A basic description of EPACS can be found in the LANSCE 2000 Activity Report at http://lansce.lanl.gov/news/ARtabofContents.htm.) The support infrastructure that was put in place consists of a collection of electrical boxes and racks that contain the shutter controls, the key release node, the EPACS interface, and the data-collection and communications equipment for the shutters and EPACS. The old mercury shutters were removed along with their controls, and the new sealed shutters were put in place. EPACS was designed with this application in mind and contains all the shutter and access controls.

We performed extensive planning in 2001 to ensure that installation projects for the flight paths (FPs) at Lujan Center could be accomplished during the extended maintenance period in early 2002. These installation projects will include new EPACS and shutter controls for the eight old mercury shutters (FP1, 3, 5, 6, 7, 8, 9, and 16), the two old mechanical shutters (FP10 and 11), and the two new mechanical shutters (FP12 and 13). This work will complete the EPACS and shutter-control installation at Lujan Center.

↑ ***Fig. 1.*** *New EPACS and shutter-control installation at the Lujan Center.*

Weapons Neutron Research Facility Upgrades

The old Personnel Safety System for the WNR Target 2 and Target 4 was removed, and the configuration of the WNR South Yard (Fig. 2) was revised and incorporated into a new five-zone EPACS system called "WNR Target 2/4 Exclusion Area." Zone 1 includes the area to the northeast of building MPF-29 up to Target 4. Zone 2 contains most of the shutters and collimators for Target 4 and allows convenient access by the experiments to the collimators. Zone 3 replaces the area controlled by the old South Yard key in front of the access to the Target 4 tunnel. Zone 4 is the roof of Target 4, and Zone 5 is the area around Target 2. Careful layout of Zone 5 eliminates the need to enter the fenced area to do a sweep and reduces the chance of a falling hazard in that very rugged terrain.

↑ ***Fig. 2.*** *The new EPACS installation in WNR's South Yard.*

↑ ***Fig. 3.*** *EPACS installation in the new ICE House.*

EPACS for the New Irradiation of Chips and Electronics Facility

The EPACS system for the ICE House (Fig. 3) was designed and installed in a very short period of time to allow industrial users on-time access to the neutron beam. The entire experimental area went from a bare patch of dirt to production in less that 60 days. The EPACS system was the very last item to be installed and was brought on line over a record two-day period. Johnson Controls of Northern New Mexico installed the necessary gutters and conduit runs, and the LANSCE-6 Protective Systems Team was then able to install the hardware and cables, complete the wiring, and get the procedures ready for the final interlock checks.

New Irradiation of Chips and Electronics Facility Highlights 2001 Infrastructure Improvements

The days of bending under beam pipes and wading through mud puddles to get to their experiments are over for many scientists working on single-event-effects (SEE) studies at the Weapons Neutron Research Facility (WNR). Construction of the new Irradiation of Chips and Electronics (ICE) House began in July 2001 and serviced its first customers in September. This bright new building (Fig. 1), located on the 30°L flight path (FP) at WNR, is a welcome haven to many researchers who in the past had to hike from Building 7 to two tiny sheds (Fig. 2), braving the weather and ducking under steel pipes, to perform their experiments. Now the experimenters can drive right up to the building on a new asphalt road to unload their equipment, a change that will surely elate previous users not used to such "luxury." The new road is also a great boon to WNR technicians who previously had to dismantle other FPs to move in experimental equipment for the SEE studies. Not only can the scientists now stay dry and spare their backs, they have a place approximately three times bigger to perform their experiments. The ICE House is equipped with an overhead crane and rollup door to facilitate setting up experimental apparatus. The facility has separate experimental, diagnostic, and control areas all under the same roof. Lined with concrete shielding blocks, the experimental area (Fig. 3) receives beam from Target 4 of the WNR. Researchers set up their experiments in this area with the help of alignment lasers. On the other side of the shielding wall is the diagnostic area where experimenters can set up computers and other diagnostic equipment to record

↑ ***Fig. 2.*** *Previous home of the single-event effects experiments. On top is the old irradiation shed. The building on the bottom was used for diagnostics and experiment data-acquisition equipment.*

↑ ***Fig. 1.*** *ICE House, new home of SEE experiments conducted at the WNR.*

↑ ***Fig. 3.*** *Photo of Prairie View A&M University personnel setting up a typical small-scale experiment in the new irradiation area. The shield wall behind them protects the diagnostic and controls areas shown below.*

↑ ***Fig. 4.*** *Researchers from Honeywell take data in the diagnostic area.*

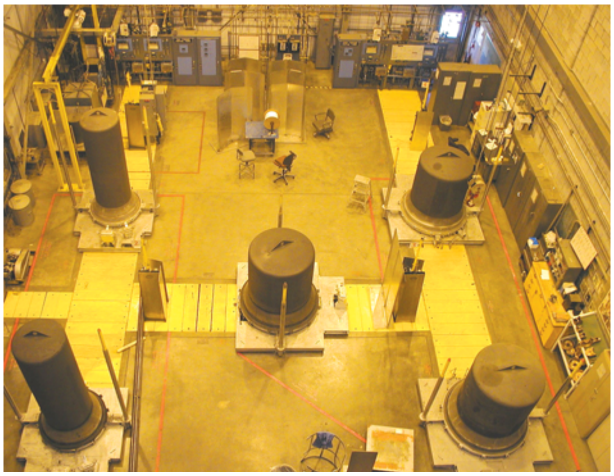
their data (Fig. 4). Adjacent to the diagnostic area is the controls area where LANSCE-3 personnel monitor the delivered neutron spectrum.

The intensity and shape of the neutron spectrum produced at the Los Alamos Neutron Science Center (LANSCE) gives the ICE House a capability unique in the world for conducting neutron-induced SEE research. LSI Logic Corporation had the honor of christening the facility as its first user in September. Since then, Honeywell, Intel, and Altera were among the record number of SEE experimenters that LANSCE was able to accommodate during the 2001 run cycle. A record number of proposals is anticipated in 2002 as awareness of the new facility spreads. For information on the experiments conducted at the ICE House, see the highlight article *Single-Event Effects Measurements at the LANSCE Irradiation of Chips and Electronics House* on p. 80 of this report.

– Bruce Takala

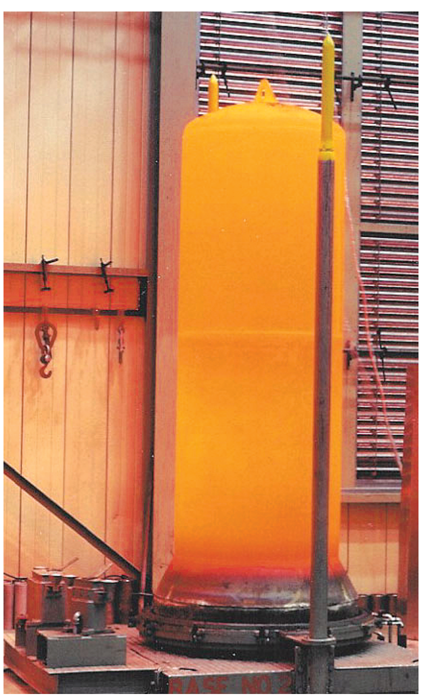
Hydrogen-Brazing-Furnace Operations

The Los Alamos Neutron Science Center (LANSCE) operates and maintains an industrial gas-atmosphere-furnace facility, which was first assembled to fabricate the Los Alamos Meson Physics Facility (LAMPF)/LANSCE accelerator in the late 1960s. The facility (Fig. 1) consists of two large electric furnaces and five workstations covered with high-temperature, high-strength steel Inconel-600 retorts. A retort is a vessel that is either under vacuum during purging operations or contains a pure atmosphere at brazing temperatures. Brazing is the physical bonding of two parent materials by the melting of a third material before they melt. This process is distinguished from soldering in that it is a relatively high-temperature operation [(i.e., greater than 450°C (840°F)].



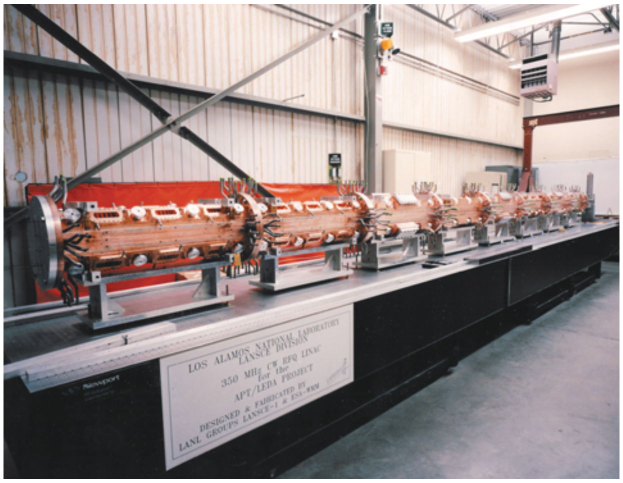
↑ ***Fig. 1.*** *Furnace facility showing five retort work stations and control panels.*

The furnaces may be operated with either catalytically dried hydrogen or argon atmospheres up to 1,093°C (2,000°F) (Fig. 2). The electric furnaces and retorts are of two different sizes and will accommodate relatively large workloads up to 1,814 kg (4,000 lb) each. The tall furnace will accept parts as large as 0.76-m (30-in.) diameter by 2.13-m (84-in.) high. The short furnace will accept parts as large as 1.27-m (50-in.) diameter by 0.94-m (37-in.) high. A typical tall furnace load can be seen in Fig. 3. An independent 6,818-kg (7.5-ton) overhead crane serves each furnace. When fully staffed, the facility can conduct brazing operations and set-up sequences simultaneously.



↑ ***Fig. 2.*** *Tall retort immediately after furnace removal.*

↑ ***Fig. 3.*** *Stack-braze assembly for the LAMPF/LANSCE 805-MHz side-coupled linear accelerator.*



↑ ***Fig. 4.*** *APT radio-frequency quadruple brazed at LANSCE.*

The furnace facility continues to meet the need for brazing new accelerators (Fig. 4) and accelerator-replacement components, for klystron-tube re-building, and for support of experiment needs for special apparatuses best assembled by gas-atmosphere-furnace-brazing techniques.

— *Michael Borden*

Cooling Tower Replacement Project

During compliance sampling in 1996, National Pollutant Discharge Elimination System (NPDES) permit levels for arsenic in the Los Alamos Neutron Science Center (LANSCE) cooling tower basins were exceeded and reported to the Environmental Protection Agency (EPA). Wood slats treated with arsenic-based preservative within the cooling towers were determined to be the source of the arsenic. To address the NPDES non-compliance, we halted normal blow-down discharges. New ion exchange columns were installed at the site as an interim corrective action, and water from the cooling towers was routed through them to remove the arsenic. Operational samples were collected from cooling-tower basins. Once analytical results showed the arsenic levels in compliance with NPDES permit requirements, the ion exchange columns were removed from service and normal tower operations resumed. Los Alamos National Laboratory advised EPA in a letter dated February 14, 1997 (Los Alamos National Laboratory letter, ESH-18/WQ&H:97-0053) that long-term corrective actions included replacement of the cooling towers and that, subject to DOE funding approval, the completion for construction of two new cooling towers was estimated to be April 1998. This schedule was revised by a letter dated June 28, 2000, changing the estimated completion date for replacement of all the cooling towers to March 2002. Three independent cooling towers and cooling-water distribution systems support the linear accelerator (linac) at LANSCE. Each cooling tower and its associated distribution system constitutes a complete and useable facility. Cooling tower 53-60 and its distribution system serves the injector end of the accelerator. Tower 53-62 serves the main linac portion of the accelerator (sectors B through H), which is the largest and most critical section. Cooling tower 53-64 provides cooling water to the switchyard, Area A, the PSR, WNR experimental areas, and the Lujan Center. All of these cooling towers were constructed during the initial construction of the accelerator (1969-1971).

Currently we are operating TA-53's cooling towers in two different modes. During accelerator operations when there is a large heat load on the cooling towers, "blow down" is controlled by conductivity. During maintenance periods while the accelerator is shut off and heat loads are lower, cooling towers have a constant blow down or bleed rate—both terms relate to the discharge of water that can no longer be recycled through the cooling system of the accelerator. In this case, the water is discharged to an outfall to the environment and monitored closely for arsenic and chlorine levels. Our site operators are continuing to collect operations samples to monitor arsenic levels, and the ion-exchange columns are retained onsite as back-up treatment units.

Upon exceeding outfall arsenic permit limits, we developed an iterative replacement program and made commitments to EPA with the first tower to be replaced in

Fig. 1. *Cooling Tower 53-978 (53-64 replacement) in the foreground and Cooling Tower 53-963 (53-60 and 53-62 replacement) in the background.*

fiscal year (FY) 1998. The second cooling tower was scheduled for completion in FY2000 and the third in FY2001. The planned approach for replacement of the towers was to construct a replacement tower and service building immediately adjacent to each of the existing towers. Although the original schedule has been delayed, our commitment to replace the towers remains the same. We have kept the New Mexico Environmental Department abreast of the status change, and they have been supportive to date. The first of the projects—replacement of Cooling Tower 53-62—was completed in April 2001. The replacement tower is commissioned and is fully operational. This project was revised to extend the distribution system to the injector end of the accelerator, thereby eliminating the need for Cooling Tower 53-60. Tower 53-60 has been disconnected and will be torn down in FY2002. The Engineering Study and Title II Design for the replacement for Tower 53-64 were completed in FY2000. The construction contract was awarded in April 2000 and was completed in December 2001 (Fig. 1). The new tower will be fully operational in January 2002. Demolition of the three old towers, 53-60, 53-62, and 53-64, is scheduled to begin on March 11, 2002, and will be complete by May 1, 2002.

The new cooling tower is constructed on a concrete tower basin that matches the footprint of the new tower. To avoid the issues associated with the existing tower, the new tower is an induced draft, counter flow, multiple cell tower that was erected on site. All components are fiberglass with type 316 stainless-steel appurtenances. The ladders and guardrails are galvanized steel. Fill material is a high-efficiency cellular-fiber type formed from Polyvinyl Chloride (PVC), with two fill-pack layers maximum.

All of these projects are being managed as a successful team effort between LANSCE Facility Management, the Nuclear Weapons Program Office, and the Project Management Division.

– Troy Belyeu

Ongoing Improvements in LANSCE 1L Target Facility Operation

LANSCE-7 was given responsibility for all aspects of the maintenance, improvement, and operational readiness of the Lujan Neutron Scattering Center (Lujan Center) spallation-neutron source at the Los Alamos Neutron Science Center (LANSCE) in December 1997. The spallation source, known as the 1L Target Facility, is a high-power (up to 160 kW) facility that produces fast neutrons from proton-beam interactions with tungsten and then thermalizes them to low energy in moderators surrounding the tungsten targets. The radionuclide accumulation in the targets bombarded by protons caused the spallation-neutron source to be considered "category 3 nuclear" at about the same time that LANSCE-7 assumed responsibility for its operation. The 1L Target Facility includes the components that produce the neutrons (e.g., targets, moderators, and reflectors) and the systems that support the operation of these components (shielding, closed-loop cooling water, vacuum, cryogenic helium and hydrogen, instrumentation, and interlocks and controls).

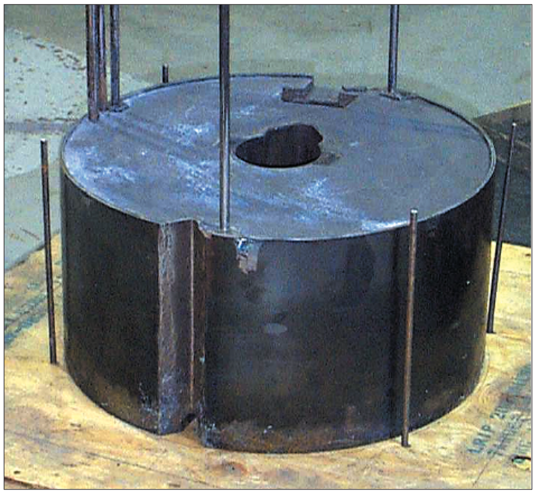
During 2001, the 1L Target Facility ran with a 99.16% availability (i.e., the facility was available except for 23 out of the 2,735 scheduled hours), which was an improvement over the 97.26% availability of 2000. The enhanced reliability was the result of two improvements made early in the year: (1) completing the cadre of formally qualified 1L Target Facility Operators and (2) redesigning the 1L Target cooling water systems to properly remove gas produced through radiolysis of water.

The additional qualified operators allowed more effort (and more eyes) to be applied toward the long-term tracking and trending of the 1L Target and support system performance. (Most of the system components are highly radioactive, embedded in shielding, and can only be evaluated indirectly.) The trending program resulted in the discoveries of the gradual loss of cooling to a lead reflector and to one of the two tungsten targets.

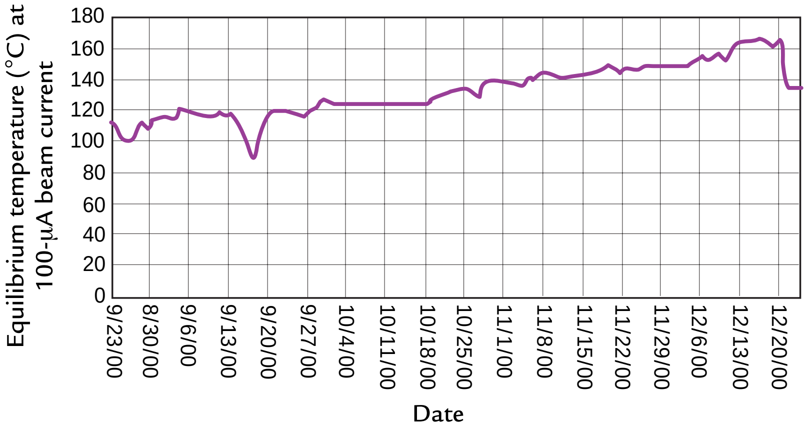
1L Target Improvements

Fig. 1 shows the 1L Target lower lead reflector, which is cooled by water flowing through stainless-steel tubing embedded in the lead. Fig. 2 is a plot of the equilibrium temperature of this reflector over time. The increase in temperature came from of a loss in thermal contact between the cooling tubes and the lead.

Fig. 3 shows the upper tungsten target during assembly, including the cooling water supply (upper) and return (lower) tubes. Fig. 4 is a plot of the flow conductance through this target assembly over time. The plot demonstrates a steadily lowering resistance to cooling-water flow, which was postulated to be caused by an internal weld failure whereby cooling water partially bypassed the tungsten in the target module by leaking directly from the supply tube to the return tube. Both these problems resulted in the loss of cooling capacity to the large, complex target assembly. However, by trending the performance of the target and support systems, we identified the deficiencies before components were seriously damaged and established additional controls to support continued safe target operation.



↑ Fig. 1. *1L Target lower lead reflector.*



↑ Fig. 2. *1L Target lower-lead-reflector temperature versus time.*

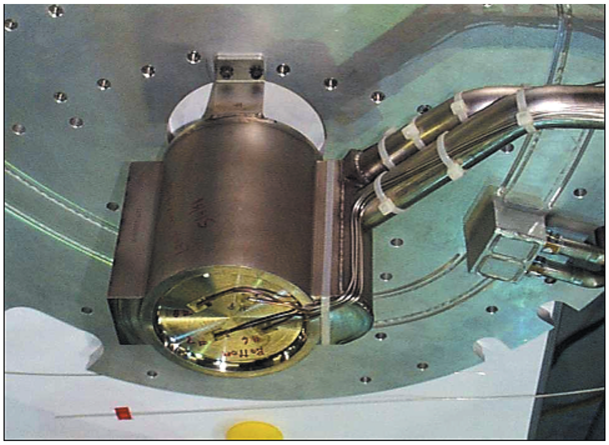


Fig. 3. *1L upper tungsten target.*

The second significant improvement was redesigning 1L Target cooling-water systems to properly remove gas produced through radiolysis of water. Normal beam interactions with water produce hydrogen and oxygen. Some of this gas will recombine to form other solutions, but the rest must be continuously removed from the system to avoid pressure buildup.[1] During the CY 2000, beam delivery was suspended to the 1L Target for about an hour each day to manually vent these gases because the 1L Target water systems were not properly designed to automatically do it. The net gas production measured in the most highly irradiated water system was about one mole of gas per day at 100 μA of proton-beam current. During the 2001 outage for accelerator maintenance, cyclonic air eliminators suitable for the application were installed in the 1L Target water systems (Fig. 5). The air eliminators were a success, and beam delivery was not suspended for venting gas during 2001.

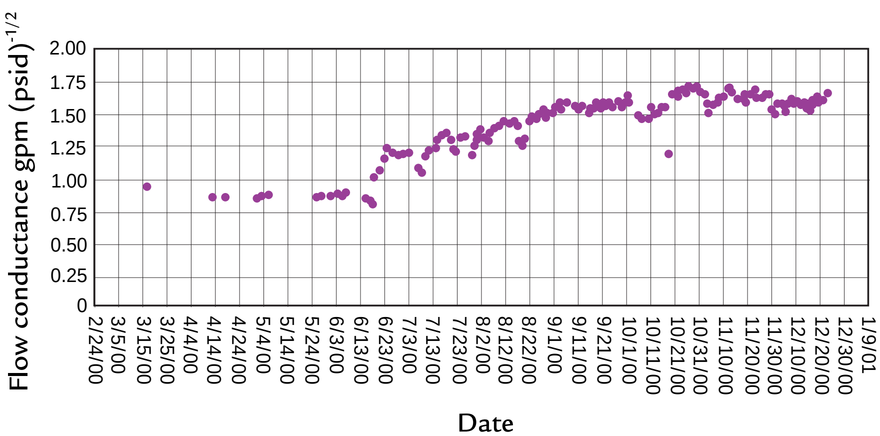


Fig. 4. *Upper-target conductance versus time.*

Fig. 5. *Cyclonic air separators.*

Conclusion

The 1L Target Facility experienced very reliable operation in 2001 in large part because of the successful qualification of additional operators and the new designs that eliminated the need to periodically suspend beam delivery. The examples provided in this article illustrate just a few of the ways continuous improvement in the operation of the 1L Target Facility was achieved.

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– Mike Baumgartner

LANSCE-1 Superconducting Laboratory—Improved Capability in Handling Superconducting Accelerating Structures

Superconducting (SC) accelerating cavities made of niobium or niobium-coated copper have become prevalent throughout the world during the past 15 years because of their high gradients and energy efficiency as compared to conventional copper cavities. The technology required to successfully apply these SC cavities necessitated many facility improvements to clean the cavity inner surface and avoid contamination, which is detrimental to the performance of the cavity. This article describes the upgraded facilities in MPF-17 at the Los Alamos Neutron Science Center (LANSCE), which include a class-100 clean room, an ultra-pure-water system, and a high-pressure rinsing system. Some results obtained with these SC cavities are also discussed.

Facilities

Clean assembly is one of the most important factors for the success of SC cavity technology because micron-size particles can deteriorate the cavity performance. LANSCE-1 personnel in the SC Laboratory at MPF-17 have been upgrading the facilities to meet the needs of clean-cavity assembly.

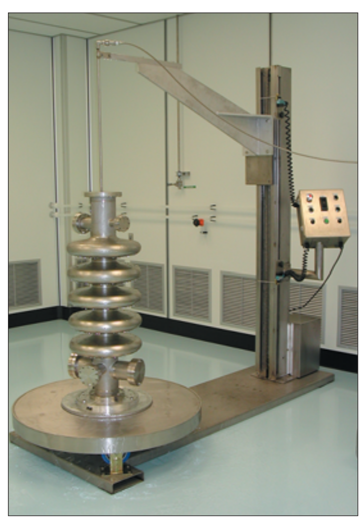
Figs. 1 and 2 show a 2,600-ft^2 clean room and an ultra-pure water system. These facilities were built to treat 700-MHz five-cell SC cavities originally planned for the high-energy linear accelerator (linac) sections of the Accelerator Production of Tritium (APT) project. These facilities allow assembly of a cryostat module housing two APT cavities, four high-power input couplers in a very clean environment.[1,2]

↑ *Fig. 1. This 2,600-ft^2 clean room is divided into class-1,000 and class-100 clean rooms for assembling SC cavities. "Class-N" means less than N particles larger than 0.5 micron per cubic feet.*

↑ *Fig. 2. Ultra-pure water system that can produce 2,000 gallons per day of de-ionized water with a resistivity (purity) of > 18 MΩ·cm. Shown in the center is a 1,500-gallon storage tank.*

In 2001, we installed two new facilities: a new high-pressure rinsing system and a new ultrasonic cleaning system. Fig. 3 shows the new high-pressure, ultra-pure-water rinsing station with an APT five-cell SC cavity. While the cavity is rotating on a round table, water jets at 1,000 psi rinse chemical residues and particles from the inner surface of the cavity. This new station will also accommodate a cavity with an outer helium vessel.

Fig. 4 shows a new ultrasonic cleaning station, which consists of three 90-gallon baths—one is for degreasing



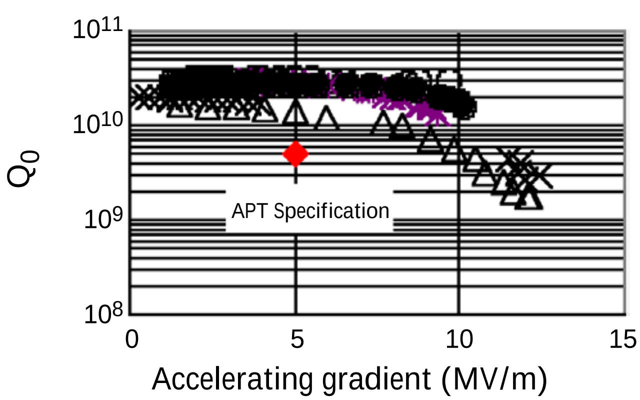
← *Fig. 3. New high-pressure rinsing system with a 700-MHz, five-cell APT-type cavity. While the cavity is rotating on the turn table at ~ 30 rpm, water jets at ~ 1,000 psi move up and down automatically and rinse off the particles and chemical residues from the inner surface of the cavity.*

↑ *Fig. 4. Ultrasonic cleaning system to degrease, clean, and rinse the components for SC cavities and power couplers. The system consists of three 90-gallon baths with 40-kHz oscillators. This system is installed in the Class-1,000 clean room.*

and coarse cleaning with a detergent, and the other two are for rinsing. The main purpose of this station is to clean high-power input couplers, although this has not yet been carried out because of a stoppage of the coupler work.

SC Cavity Test Results

Using these facilities, we have treated APT five-cell cavities and one spoke cavity on loan from Argonne National Laboratory.[3-5] Fig. 5 shows the quality factor, Q_0, which is inversely proportional to the surface loss as a function of accelerating gradient of five prototype APT 700-MHz, five-cell cavities. The design



↑ *Fig. 5. Results of performance tests of five β = 0.64, 700-MHz, five-cell APT cavities. Plotted are the cavity quality factors Q_0 (larger values imply less loss in the cavity) as a function of accelerating gradient. All the cavities exceeded the APT specification (red diamond) with ample margin.*

requirement of the APT project (shown with a red-diamond designation) is $Q_0 = 5 \times 10^9$ at an accelerating field of 5 MV/m. As shown in Fig. 5, we exceeded the requirement by more than 100%, i.e., the surface losses and accelerating gradients of most cavities were better by a factor of > 2.

Future Infrastructure Upgrades

Many other laboratories involved in SC cavity work have installed chemical or electrolytic etching and polishing facilities in their clean rooms to reduce the chance of contamination. The installation of these facilities in the clean room will be our next step at LANSCE. Additionally, a pumping unit and a leak-detector system will be installed in the clean room to permit re-assembly of cavities without contamination.

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– Tsuyoshi Tajima